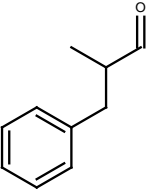


Query

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Reaxys ID 2042984 View in Reaxys		1/3
		<p>Chemical Name: 3-phenyl-2-methylpropionaldehyde; 2-methyl-3-phenylpropanal; phenyl-2-propyl ketone; 2-methyl-3-phenylpropionaldehyde; 1-phenyl-2-methylpropanal; 2-benzylpropionaldehyde; 2-methyl-3-phenyl-propionaldehyde</p> <p>Molecular Formula: C₁₀H₁₂O</p> <p>CAS Registry Number: 5445-77-2; 42307-59-5; 63262-79-3; 78964-59-7</p> <p>Molecular Weight: 148.205</p> <p>Linear Structure Formula: HCOCH(CH₃)CH₂(C₆H₅)</p> <p>Type of Substance: isocyclic</p> <p>InChIKey: HEPHYCJJLAUKSB-UHFFFAOYSA-N</p> <p>Note:</p>
Substance Label (24)		
Label	References	
Tab 2, aldehyde, run 22	Iwanami, Katsuyuki; Yano, Kentaro; Oriyama, Takeshi; Chemistry Letters; vol. 36; nb. 1; (2007); p. 38 - 39, View in Reaxys	
10c	Calo, Vincenzo; Nacci, Angelo; Monopoli, Antonio; Ferola, Valentina; Journal of Organic Chemistry; vol. 72; nb. 7; (2007); p. 2596 - 2601, View in Reaxys	
XX	Tijani, Jimoh; Ali, Bassam El; Journal of Organometallic Chemistry; vol. 692; nb. 16; (2007); p. 3492 - 3497, View in Reaxys	
1	Larsson, Michael; Hoegberg, Hans-Erik; Tetrahedron; vol. 57; nb. 35; (2001); p. 7541 - 7548, View in Reaxys ; Kim, Sung-Gon; Park, Tae-Ho; Tetrahedron Letters; vol. 47; nb. 51; (2006); p. 9067 - 9071, View in Reaxys	
carbonyl comp. tab 2/2	Iwanami, Katsuyuki; Aoyagi, Masaru; Oriyama, Takeshi; Tetrahedron Letters; vol. 47; nb. 27; (2006); p. 4741 - 4744, View in Reaxys	
4l	Reetz, Manfred T.; Guo, Hongchao; Synlett; nb. 13; (2006); p. 2127 - 2129, View in Reaxys	
T.1.E.7.Aldehyde 2.	Abu-Reziq, Raed; Avnir, David; Blum, Jochanan; European Journal of Organic Chemistry; nb. 17; (2005); p. 3640 - 3642, View in Reaxys	
4, Tab. 4, entry 6	Seiche, Wolfgang; Schuschowski, Alexander; Breit, Bernhard; Advanced Synthesis and Catalysis; vol. 347; nb. 11-13; (2005); p. 1488 - 1494, View in Reaxys	
Tab. 2, entry 9, prod.	Mhadgut, Shilpa C.; Palaniappan, Kumaranand; Thimmaiah, Muralidhara; Hackney, Stephen A.; Toer-oek, Bela; Liu, Jian; Chemical Communications (Cambridge, United Kingdom); nb. 25; (2005); p. 3207 - 3209, View in Reaxys	
4j	Benati, Luisa; Leardini, Rino; Minozzi, Matteo; Nanni, Daniele; Scialpi, Rosanna; Spagnolo, Piero; Zannardi, Giuseppe; Synlett; nb. 6; (2004); p. 985 - 990, View in Reaxys	
Product, Tab.2, run 6	Lee, Hee-Yoon; An, Mihyun; Tetrahedron Letters; vol. 44; nb. 14; (2003); p. 2775 - 2778, View in Reaxys	
Tab1run7; product (β)	Calo, Vincenzo; Nacci, Angelo; Monopoli, Antonio; Spinelli, Michele; European Journal of Organic Chemistry; nb. 8; (2003); p. 1382 - 1385, View in Reaxys	
ent-30/30	Bull, Steven D.; Davies, Stephen G.; Nicholson, Rebecca L.; Sanganee, Hitesh J.; Smith, Andrew D.; Organic and Biomolecular Chemistry; vol. 1; nb. 16; (2003); p. 2886 - 2899, View in Reaxys	
41	Bach, Jordi; Blachere, Cecile; Bull, Steven D.; Davies, Stephen G.; Nicholson, Rebecca L.; Price, Paul D.; Sanganee, Hitesh J.; Smith, Andrew D.; Organic and Biomolecular Chemistry; vol. 1; nb. 12; (2003); p. 2001 - 2010, View in Reaxys	
2	Roda, Gabriella; Riva, Sergio; Danieli, Bruno; Griengl, Herfried; Rinner, Uwe; Schmidt, Michael; Zabelinskaja, Antonina Mackova; Tetrahedron; vol. 58; nb. 15; (2002); p. 2979 - 2984, View in Reaxys	
7aa	Oi, Shuichi; Moro, Mitsutoshi; Ito, Hisanori; Honma, Yoshio; Miyano, Sotaro; Inoue, Yoshio; Tetrahedron; vol. 58; nb. 1; (2002); p. 91 - 98, View in Reaxys	
6c/6d	Tyrrell, Elizabeth; Skinner, George A.; Janes, John; Milsom, Greig; Synlett; nb. 7; (2002); p. 1073 - 1076, View in Reaxys	
10	Hosokawa, Takahiro; Kamiike, Taisuke; Murahashi, Shun-Ichi; Shimada, Mamoru; Sugafuji, Toshihiro; Tetrahedron Letters; vol. 43; nb. 51; (2002); p. 9323 - 9326, View in Reaxys	
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table 1, entry 9	Zhao, Hong; Cai, Ming-Zhong; Hu, Rong-Hua; Song, Cai-Sheng ; Synthetic Communications; vol. 31; nb. 23; (2001); p. 3665 - 3670, View in Reaxys			
2f	Bouquillon, Sandrine; Ganchegui, Benjamin; Estrine, Boris; Henin, Francoise; Muzart, Jacques ; Journal of Organometallic Chemistry; vol. 634; nb. 2; (2001); p. 153 - 156, View in Reaxys			
3c	Matoba, Kazutaka; Motofusa, Shin-ichi; Cho, Chan Sik; Ohe, Kouichi; Uemura, Sakae ; Journal of Organometallic Chemistry; vol. 574; nb. 1; (1999); p. 3 - 10, View in Reaxys			
14, R=Me	Bach, Jordi; Bull, Steven D.; Davies, Stephen G; Nicholson, Rebecca L.; Sanganee, Hitesh J.; Smith, Andrew D. ; Tetrahedron Letters; vol. 40; nb. 36; (1999); p. 6677 - 6680, View in Reaxys			
5d	Orru, Romano V. A.; Mayer, Sandra F.; Kroutil, Wolfgang; Faber, Kurt ; Tetrahedron; vol. 54; nb. 5-6; (1998); p. 859 - 874, View in Reaxys			
Patent-Specific Data (1)				
Location in Patent	References			
Claim	Patent; Helene Curtis, Inc. ; US5554363; (1996); (A1) English, View in Reaxys			
Crossfile Reference (3)				
Data Type	Name	Crossfile Source	External Access ID	References
	2-methyl-3-phenylpropionaldehyde	EINECS	226-654-9	Beilstein Handbook , View in Reaxys
Middle-IR Peaklist	A-METHYL-HY-DROCINNAMAL-DEHYDE	SpecInfo Database	STCC-75675-325 T	Unpublished , View in Reaxys
13C-NMR Spectrum	A-METHYL-HY-DROCINNAMAL-DEHYDE	SpecInfo Database	STCC-75675-325 T	Unpublished , View in Reaxys
Related Structure (1)				
Related Structure	References			
In dem H 316 beschriebenen Praeparat von Darzens hat (+)-2-Methyl-4-phenyl-butyraldehyd vorgelegen.	Hanley et al. ; Journal of Organic Chemistry; vol. 23; (1958); p. 1461,1462, View in Reaxys			
Derivative (11)				
Comment	Derivative	References		
	2-methyl-3-phenyl-propionaldehyde-(2,4-dinitrophenylhydrazone)	Petrier, Christian; Barbosa, Jayne C. de Souza; Dupuy, Claude; Luche, Jean-Louis ; Journal of Organic Chemistry; vol. 50; nb. 26; (1985); p. 5761 - 5765, View in Reaxys		
Semicarbazone: F= 123grad		Patent; Rhone-Poulenc ; DE1145161; (1963); Chem.Abstr.; vol. 59; nb. 9900d; (1963), View in Reaxys		
2,4-DNP: F= 119grad		Patent; Rhone-Poulenc ; DE1145161; (1963); Chem.Abstr.; vol. 59; nb. 9900d; (1963), View in Reaxys		
Semicarbazone: F: 123grad		Patent; Rhone-Poulenc ; DE1145161; (1963); Chem.Abstr.; vol. 59; nb. 9900d; (1963), View in Reaxys		
2,4-DNP: F: 119grad		Patent; Rhone-Poulenc ; DE1145161; (1963); Chem.Abstr.; vol. 59; nb. 9900d; (1963), View in Reaxys		
2,4-Dinitrophenylhydrazon : F: 118-120grad		Patent; Simes S.p.A. ; BE629257; (1962); Chem.Abstr.; vol. 63; nb. 6918c; (1965), View in Reaxys		
2,4-Dinitrophenylhydrazon, F: 120-121grad		Nagase ; Nippon Kagaku Zasshi; vol. 81; (1960); p. 938,941; Chem.Abstr.; vol. 56; nb. 1441; (1962), View in Reaxys		
2,4-dinitro-phenylhydrazone(mp:		Normant; Crisan ; Bulletin de la Societe Chimique de France; (1959); p. 463, View in Reaxys		

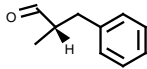
120 degree Celsius)			
2,4-dinitro-phenyl-hydrazone (mp: 119 degree)			Weizmann et al. ; Chemistry and Industry (London, United Kingdom); vol. 15; (1937); p. 587,589, View in Reaxys
semicarbazone (mp: 123 degree)			Ramart-Lucas; Labaune ; Annales de Chimie (Cachan, France); vol. <10> 16; (1931); p. 276,298, View in Reaxys
semicarbazone (mp: 70-72 degree)			Darzens ; Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences; vol. 139; (1904); p. 1216; Chem. Zentralbl.; vol. 77; nb. II; (1906); p. 1297,1298, View in Reaxys ; Patent; Darzens ; DE174239, View in Reaxys
Boiling Point (24)			
Boiling Point [°C]	Pressure [Torr]	Comment	References
129 - 130	19		Dumpis, M. A.; Kudryashova, N. I.; Veresova, M. A. ; Journal of Organic Chemistry USSR (English Translation); vol. 25; nb. 7.2; (1989); p. 1332 - 1337; Zhurnal Organicheskoi Khimii; vol. 25; nb. 7; (1989); p. 1477 - 1482, View in Reaxys
83	4		Kikukawa, K.; Nagira, K.; Wada, F.; Matsuda, T. ; Tetrahedron; vol. 37; (1981); p. 31 - 36, View in Reaxys
55 - 60	1		Nalesnik, Theodore E.; Freudenberg, John H.; Orchin, Milton ; Journal of Organometallic Chemistry; vol. 221; nb. 2; (1981); p. 193 - 198, View in Reaxys
106 - 109	25		Patent; Louisiana Univ. ; US4131623; (1978); Chem.Abstr.; vol. 90; nb. 103418, View in Reaxys
51 - 54	0.05		Comins; Meyers ; Synthesis; (1978); p. 403, View in Reaxys
96	10		Chalk; Magennis ; Journal of Organic Chemistry; vol. 41; (1976); p. 273,274,275,276,278, View in Reaxys
107 - 113	14		Melpolder, J.B.; Heck, R.F. ; Journal of Organic Chemistry; vol. 41; nb. 2; (1976); p. 265 - 272, View in Reaxys
120 - 124	3		Schwenker, G. ; Synthesis; (1975); p. 496 - 499, View in Reaxys
75 - 85	3		Heck ; Organic Syntheses; vol. 51; (1971); p. 17,19, View in Reaxys
77 - 80	3		Heck ; Organic Syntheses; vol. 51; (1971); p. 17,19, View in Reaxys
71 - 75	3		Heck ; Journal of the American Chemical Society; vol. 90; (1968); p. 5538, View in Reaxys
95 - 96	10		Abe; Yasukawa ; Yuki Gosei Kagaku Kyokaishi; vol. 22; (1964); p. 209; Chem.Abstr.; vol. 60; nb. 13175, View in Reaxys
65 - 66	10		Patent; Soda Aromatic Co. ; NL6502482; (1964); Chem.Abstr.; vol. 64; nb. 19497g; (1966), View in Reaxys
89 - 90	6		Urry, W.H. et al. ; Journal of Organic Chemistry; vol. 29; nb. 7; (1964); p. 1663 - 1669, View in Reaxys
110 - 112	16		Ferrari, G.; Casagrande, C. ; Farmaco, Edizione Scientifica; vol. 18; (1963); p. 780 - 792, View in Reaxys
92	6		Scrabine, I. ; Bulletin de la Societe Chimique de France; (1961); p. 1194 - 1198, View in Reaxys ; Patent; Rhone-Poulenc ; DE1145161; (1963); Chem.Abstr.; vol. 59; nb. 9900d; (1963), View in Reaxys
93 - 96	3		Nagase ; Nippon Kagaku Zasshi; vol. 81; (1960); p. 938,941; Chem.Abstr.; vol. 56; nb. 1441; (1962), View in Reaxys
226 - 227	760		Malinovskii, M.S.; Yudasina, A.G. ; J. Gen. Chem. USSR (Engl. Transl.); vol. 30; nb. 6; (1960); p. 1831 - 1837,1814 - 1820, View in Reaxys
109 - 111	16		Normant; Crisan ; Bulletin de la Societe Chimique de France; (1959); p. 463, View in Reaxys
108 - 109	12		Shinya ; Nippon Noge Kagaku Kaishi; vol. 29; (1955); p. 91,92; Chem.Abstr.; (1959); p. 1227, View in Reaxys

90	6		Ramart-Lucas; Labaune ; Annales de Chimie (Cachan, France); vol. <10> 16; (1931); p. 276,298, View in Reaxys
129 - 130	19		Darzens ; Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences; vol. 139; (1904); p. 1216; Chem. Zentralbl.; vol. 77; nb. II; (1906); p. 1297,1298, View in Reaxys ; Patent ; Darzens ; DE174239, View in Reaxys
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227 - 228			Patent ; Behal; Sommelet ; DE177614, View in Reaxys
Refractive Index (8)			
Refractive Index	Wavelength [nm]	Temperature [°C]	References
1.5141	589	20	Urry, W.H. et al. ; Journal of Organic Chemistry; vol. 29; nb. 7; (1964); p. 1663 - 1669, View in Reaxys ; Dumpis, M. A.; Kudryashova, N. I.; Veresova, M. A. ; Journal of Organic Chemistry USSR (English Translation); vol. 25; nb. 7.2; (1989); p. 1332 - 1337; Zhurnal Organicheskoi Khimii; vol. 25; nb. 7; (1989); p. 1477 - 1482, View in Reaxys
1.5113	589	25	Heck ; Organic Syntheses; vol. 51; (1971); p. 17,19, View in Reaxys
1.511	589	20	Malinovskii, M.S.; Yudasina, A.G. ; J. Gen. Chem. USSR (Engl. Transl.); vol. 30; nb. 6; (1960); p. 1831 - 1837, 1814 - 1820, View in Reaxys ; Abe; Yasukawa ; Yuki Gosei Kagaku Kyokaishi; vol. 22; (1964); p. 209; Chem. Abstr.; vol. 60; nb. 13175, View in Reaxys ; Patent ; Soda Aromatic Co. ; NL6502482; (1964); Chem. Abstr.; vol. 64; nb. 19497g; (1966), View in Reaxys
1.5087	589	24	Patent ; Rhone-Poulenc ; DE1145161; (1963); Chem. Abstr.; vol. 59; nb. 9900d; (1963), View in Reaxys
1.5087	589	29	Scriabine, I. ; Bulletin de la Societe Chimique de France; (1961); p. 1194 - 1198, View in Reaxys
1.5141	589	23	Nagase ; Nippon Kagaku Zasshi; vol. 81; (1960); p. 938,941; Chem. Abstr.; vol. 56; nb. 1441; (1962), View in Reaxys
1.5092	589	24	Normant; Crisan ; Bulletin de la Societe Chimique de France; (1959); p. 463, View in Reaxys
1.5182	589	20	Shinya ; Nippon Noge Kagaku Kaishi; vol. 29; (1955); p. 91,92; Chem. Abstr.; (1959); p. 1227, View in Reaxys
Density of the Liquid (3)			
Density of the Liquid	Reference Temperature [°C]	Measurement Temperature [°C]	References
		20	Abe; Yasukawa ; Yuki Gosei Kagaku Kyokaishi; vol. 22; (1964); p. 209; Chem. Abstr.; vol. 60; nb. 13175, View in Reaxys ; Patent ; Soda Aromatic Co. ; NL6502482; (1964); Chem. Abstr.; vol. 64; nb. 19497g; (1966), View in Reaxys
0.9925	4	20	Malinovskii, M.S.; Yudasina, A.G. ; J. Gen. Chem. USSR (Engl. Transl.); vol. 30; nb. 6; (1960); p. 1831 - 1837, 1814 - 1820, View in Reaxys
0.982	4	24	Normant; Crisan ; Bulletin de la Societe Chimique de France; (1959); p. 463, View in Reaxys
NMR Spectroscopy (15)			
1 of 15	Description	Chemical shifts	
	Nucleus	1H	
	Solvents	CDCl3	
	Frequency [MHz]	250	
	Oi, Shuichi; Moro, Mitsutoshi; Ito, Hisanori; Honma, Yoshio; Miyano, Sotaro; Inoue, Yoshio ; Tetrahedron; vol. 58; nb. 1; (2002); p. 91 - 98, View in Reaxys		
2 of 15	Nucleus	1H	
	Coupling Nuclei	1H	

	Solvents	CDCl ₃
	Frequency [MHz]	250
	Oi, Shuichi; Moro, Mitsutoshi; Ito, Hisanori; Honma, Yoshio; Miyano, Sotaro; Inoue, Yoshio; Tetrahedron; vol. 58; nb. 1; (2002); p. 91 - 98, View in Reaxys	
	Description	Chemical shifts
	Nucleus	¹³ C
3 of 15	Solvents	CDCl ₃
	Frequency [MHz]	62.5
	Oi, Shuichi; Moro, Mitsutoshi; Ito, Hisanori; Honma, Yoshio; Miyano, Sotaro; Inoue, Yoshio; Tetrahedron; vol. 58; nb. 1; (2002); p. 91 - 98, View in Reaxys	
	Description	Chemical shifts
	Nucleus	¹ H
4 of 15	Coupling Nuclei	¹ H
	Solvents	CDCl ₃
	Matoba, Kazutaka; Motofusa, Shin-ichi; Cho, Chan Sik; Ohe, Kouichi; Uemura, Sakae; Journal of Organometallic Chemistry; vol. 574; nb. 1; (1999); p. 3 - 10, View in Reaxys	
	Description	Chemical shifts
	Nucleus	¹ H
5 of 15	Solvents	CDCl ₃
	Frequency [MHz]	300
	Orru, Romano V. A.; Mayer, Sandra F.; Kroutil, Wolfgang; Faber, Kurt; Tetrahedron; vol. 54; nb. 5-6; (1998); p. 859 - 874, View in Reaxys	
	Nucleus	¹ H
	Coupling Nuclei	¹ H
6 of 15	Solvents	CDCl ₃
	Frequency [MHz]	300
	Orru, Romano V. A.; Mayer, Sandra F.; Kroutil, Wolfgang; Faber, Kurt; Tetrahedron; vol. 54; nb. 5-6; (1998); p. 859 - 874, View in Reaxys	
	Description	Chemical shifts
	Nucleus	¹ H
7 of 15	Solvents	CDCl ₃
	Meyers, A. I.; Walkup, Robert D.; Tetrahedron; vol. 41; nb. 22; (1985); p. 5089 - 5106, View in Reaxys; Stamm, Helmut; Sommer, Andreas; Onistschenko, Andreas; Woderer, Anton; Journal of Organic Chemistry; vol. 51; nb. 25; (1986); p. 4979 - 4983, View in Reaxys; Petrier, Christian; Barbosa, Jayne C. de Souza; Dupuy, Claude; Luche, Jean-Louis; Journal of Organic Chemistry; vol. 50; nb. 26; (1985); p. 5761 - 5765, View in Reaxys; Cho, Chan Sik; Motofusa, Shin-ichi; Ohe, Kouichi; Uemura, Sakae; Bulletin of the Chemical Society of Japan; vol. 69; nb. 8; (1996); p. 2341 - 2348, View in Reaxys	
	Description	Chemical shifts
	Nucleus	¹³ C
	Solvents	CDCl ₃
8 of 15	Cho, Chan Sik; Motofusa, Shin-ichi; Ohe, Kouichi; Uemura, Sakae; Bulletin of the Chemical Society of Japan; vol. 69; nb. 8; (1996); p. 2341 - 2348, View in Reaxys	
	Description	Chemical shifts
	Nucleus	¹³ C
	Solvents	CDCl ₃
	Spin-spin coupling constants	
9 of 15	Solvents	CDCl ₃
	Comment	¹ H- ¹ H
	Stamm, Helmut; Sommer, Andreas; Onistschenko, Andreas; Woderer, Anton; Journal of Organic Chemistry; vol. 51; nb. 25; (1986); p. 4979 - 4983, View in Reaxys; Cho, Chan Sik; Motofusa, Shin-ichi; Ohe, Kouichi; Uemura, Sakae; Bulletin of the Chemical Society of Japan; vol. 69; nb. 8; (1996); p. 2341 - 2348, View in Reaxys	
	Description	Chemical shifts
	Nucleus	¹³ C

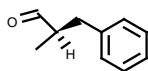
10 of 15	Description	Chemical shifts	
	Nucleus	1H	
	Meyers, A.I. et al. ; Journal of Organic Chemistry; vol. 38; (1973); p. 36 - 56, View in Reaxys ; Cho, Chan Sik; Motofusa, Shin-ichi; Ohe, Kouichi; Uemura, Sakae; Shim, Sang Chul ; Journal of Organic Chemistry; vol. 60; nb. 4; (1995); p. 883 - 888, View in Reaxys		
11 of 15	Description	Chemical shifts	
	Nucleus	13C	
	Cho, Chan Sik; Motofusa, Shin-ichi; Ohe, Kouichi; Uemura, Sakae; Shim, Sang Chul ; Journal of Organic Chemistry; vol. 60; nb. 4; (1995); p. 883 - 888, View in Reaxys		
12 of 15	Description	Spin-spin coupling constants	
	Comment	1H-1H	
	Cho, Chan Sik; Motofusa, Shin-ichi; Ohe, Kouichi; Uemura, Sakae; Shim, Sang Chul ; Journal of Organic Chemistry; vol. 60; nb. 4; (1995); p. 883 - 888, View in Reaxys		
13 of 15	Description	Chemical shifts	
	Nucleus	1H	
	Solvents	CCl4	
	Arjona, Odon; Perez-Ossorio, Rafael; Perez-Rubalcaba, Alfredo; Quiroga, Maria L. ; Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999); (1981); p. 597 - 603, View in Reaxys ; Duchene, Alain; Mouko-Mpegna, David; Quintard, Jean-Paul ; Bulletin de la Societe Chimique de France; nb. 5; (1985); p. 787 - 793, View in Reaxys		
14 of 15	Description	Spin-spin coupling constants	
	Solvents	CCl4	
	Comment	1H-1H	
	Duchene, Alain; Mouko-Mpegna, David; Quintard, Jean-Paul ; Bulletin de la Societe Chimique de France; nb. 5; (1985); p. 787 - 793, View in Reaxys		
15 of 15	Description	NMR	
	Comins; Meyers ; Synthesis; (1978); p. 403, View in Reaxys ; Kovelesky; Meyers ; Organic Preparations and Procedures International; vol. 1; (1969); p. 213, View in Reaxys ; Heck ; Organic Syntheses; vol. 51; (1971); p. 17,19, View in Reaxys ; Moss; Dolling ; Journal of the American Chemical Society; vol. 93; (1971); p. 954,955, View in Reaxys ; Heck ; Journal of the American Chemical Society; vol. 90; (1968); p. 5538, View in Reaxys		
IR Spectroscopy (8)			
Description	Solvent	Comment	References
Bands	neat (no solvent)		Oi, Shuichi; Moro, Mitsutoshi; Ito, Hisanori; Honma, Yoshio; Miya-no, Sotaro; Inoue, Yoshio ; Tetrahedron; vol. 58; nb. 1; (2002); p. 91 - 98, View in Reaxys
Bands			Meyers, A.I. et al. ; Journal of Organic Chemistry; vol. 38; (1973); p. 36 - 56, View in Reaxys ; Schwenker, G. ; Synthesis; (1975); p. 496 - 499, View in Reaxys ; Evans, John; O'Neill, Lynn; Kambhampati, Vijaya L.; Rayner, Graham; Turin, Sandra; Genge, Anthony; Dent, Andrew J.; Neisius, Thomas ; Journal of the Chemical Society, Dalton Transactions; nb. 10; (2002); p. 2207 - 2212, View in Reaxys
Bands	film		Orru, Romano V. A.; Mayer, Sandra F.; Kroutil, Wolfgang; Faber, Kurt ; Tetrahedron; vol. 54; nb. 5-6; (1998); p. 859 - 874, View in Reaxys
Bands	neat (no solvent)	3100 - 700 cm ⁻¹	Cho, Chan Sik; Motofusa, Shin-ichi; Ohe, Kouichi; Uemura, Sakae; Shim, Sang Chul ; Journal of Organic Chemistry; vol. 60; nb. 4; (1995); p. 883 - 888, View in Reaxys ; Cho, Chan Sik; Motofusa, Shin-ichi; Ohe, Kouichi; Uemura, Sakae ; Bulletin of the Chemical Society of Japan; vol. 69; nb. 8; (1996); p. 2341 - 2348, View in Reaxys
Bands		2700 - 1725 cm ⁻¹	Meyers, A. I.; Walkup, Robert D. ; Tetrahedron; vol. 41; nb. 22; (1985); p. 5089 - 5106, View in Reaxys
Bands	neat (no solvent)	3020 - 700 cm ⁻¹	Petrier, Christian; Barbosa, Jayne C. de Souza; Dupuy, Claude; Lucche, Jean-Louis ; Journal of Organic Chemistry; vol. 50; nb. 26; (1985); p. 5761 - 5765, View in Reaxys

Bands	neat (no solvent)	2800 - 1715 cm**(-1)	Arjona, Odon; Perez-Ossorio, Rafael; Perez-Rubalcaba, Alfredo; Quiroga, Maria L. ; Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999); (1981); p. 597 - 603, View in Reaxys
IR			Comins; Meyers ; Synthesis; (1978); p. 403, View in Reaxys ; Kovelsky; Meyers ; Organic Preparations and Procedures International; vol. 1; (1969); p. 213, View in Reaxys ; Moss; Dolling ; Journal of the American Chemical Society; vol. 93; (1971); p. 954,955, View in Reaxys
Mass Spectrometry (1)			
Description	References		
spectrum	Arjona, Odon; Perez-Ossorio, Rafael; Perez-Rubalcaba, Alfredo; Quiroga, Maria L. ; Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999); (1981); p. 597 - 603, View in Reaxys ; Cho, Chan Sik; Motofusa, Shin-ichi; Ohe, Kouichi; Uemura, Sakae; Shim, Sang Chul ; Journal of Organic Chemistry; vol. 60; nb. 4; (1995); p. 883 - 888, View in Reaxys ; Cho, Chan Sik; Motofusa, Shin-ichi; Ohe, Kouichi; Uemura, Sakae ; Bulletin of the Chemical Society of Japan; vol. 69; nb. 8; (1996); p. 2341 - 2348, View in Reaxys		
UV/VIS Spectroscopy (3)			
Description	Solvent	Comment	References
Spectrum		220 - 330 nm	Ramart-Lucas ; Bulletin de la Societe Chimique de France; (1950); p. 405,409, View in Reaxys
Spectrum	ethanol		Ramart-Lucas; Guilmart ; Comptes Rendus Hebdomadaires des Seances de l'Academie des Sciences; vol. 229; (1949); p. 1336, View in Reaxys
Spectrum	hexane		Ramart-Lucas; Labaune ; Annales de Chimie (Cachan, France); vol. <10> 16; (1931); p. 276,298, View in Reaxys

Reaxys ID 2500839 View in Reaxys		2/3
		<p>Chemical Name: (S)-2-methyl-3-phenylpropionaldehyde; (S)-α-methylbenzenepropanal; (R)-2-methyl-3-phenylpropanal; (S)-2-methyl-3-phenylpropanal; (2S)-(-)-2-benzyl-1-propanal</p> <p>Molecular Formula: C₁₀H₁₂O</p> <p>CAS Registry Number: 5445-77-2; 42307-59-5; 63262-79-3; 78964-59-7</p> <p>Molecular Weight: 148.205</p> <p>Linear Structure Formula: C₁₀H₁₂O</p> <p>Type of Substance: isocyclic</p> <p>InChIKey: HEPHYCJJLAUKSB-VIFPVBQESA-N</p> <p>Note:</p>
Substance Label (8)		
Label	References	
T.1. Entry 15. Substrate	Telvekar, Vikas N.; Patel, Kavita N.; Kundaikar, Harish S.; Chaudhari, Hemchandra K. ; Tetrahedron Letters; vol. 49 ; nb. 14; (2008); p. 2213 - 2215, View in Reaxys	
13	Tessier, Arnaud; Pytkowicz, Julien; Brigaud, Thierry ; Angewandte Chemie, International Edition; vol. 45 ; nb. 22; (2006); p. 3677 - 3681; Angewandte Chemie; vol. 118 ; nb. 22; (2006); p. 3759 - 3763, View in Reaxys	
30	Bull, Steven D.; Davies, Stephen G.; Nicholson, Rebecca L.; Sanganee, Hitesh J.; Smith, Andrew D. ; Organic and Biomolecular Chemistry; vol. 1 ; nb. 16; (2003); p. 2886 - 2899, View in Reaxys	
6d	Tyrrell, Elizabeth; Skinner, George A.; Janes, John; Milsom, Greig ; Synlett; nb. 7; (2002); p. 1073 - 1076, View in Reaxys	
(S)-15a	Bull, Steven D.; Davies, Stephen G.; Nicholson, Rebecca L.; Sanganee, Hitesh J.; Smith, Andrew D. ; Tetrahedron: Asymmetry; vol. 11 ; nb. 17; (2000); p. 3475 - 3480, View in Reaxys	
aldehyde a, Table 2.	Harris, Christina R.; Kuduk, Scott D.; Balog, Aaron; Savin, Ken A.; Danishefsky, Samuel J. ; Tetrahedron Letters; vol. 40 ; (1999); p. 2267 - 2270, View in Reaxys	
49i	Harris, Christina R.; Kuduk, Scott D.; Balog, Aaron; Savin, Ken; Glunz, Peter W.; Danishefsky, Samuel J. ; Journal of the American Chemical Society; vol. 121 ; nb. 30; (1999); p. 7050 - 7062, View in Reaxys	

12d	Balog, Aaron; Harris, Christina; Savin, Kenneth; Zhang, Xiu-Guo; Chou, Ting Chao; Danishefsky, Samuel J. ; Angewandte Chemie, International Edition in English; vol. 37; nb. 19; (1998); p. 2675 - 2678; Angewandte Chemie; vol. 110; (1998); p. 2821 - 2824, View in Reaxys	
Boiling Point (2)		
Boiling Point [°C]	Pressure [Torr]	References
112 - 114	20	Rangaishenvi, Milind V.; Singaram, Bakthan; Brown, Herbert C. ; Journal of Organic Chemistry; vol. 56; nb. 10; (1991); p. 3286 - 3294, View in Reaxys
80 - 100	2	Davenport et al. ; Journal of the American Chemical Society; vol. 101; (1979); p. 5654,5658, View in Reaxys
Crystal Property Description (1)		
Colour & Other Properties	References	
colourless	Chernega, Alexander N.; Davies, Stephen G.; Hepworth, David; Kurosawa, Wataru; Roberts, Paul M.; Thomson, James E.; Goodwin, Christopher J. ; Organic Letters; vol. 11; nb. 15; (2009); p. 3254 - 3257, View in Reaxys	
Optical Rotatory Power (2)		
1 of 2	Type	[alpha]
	Concentration	0.8 g/100ml
	Length of Path [cm]	10
	Solvent	chloroform
	Optical Rotatory Power [deg]	-2.8
	Wavelength [nm]	589
	Temperature [°C]	23
	Chernega, Alexander N.; Davies, Stephen G.; Hepworth, David; Kurosawa, Wataru; Roberts, Paul M.; Thomson, James E.; Goodwin, Christopher J. ; Organic Letters; vol. 11; nb. 15; (2009); p. 3254 - 3257, View in Reaxys	
2 of 2	Type	[alpha]
	Concentration	4 g/100ml
	Solvent	methanol
	Optical Rotatory Power [deg]	-4.42
	Wavelength [nm]	589
	Temperature [°C]	23
	Rangaishenvi, Milind V.; Singaram, Bakthan; Brown, Herbert C. ; Journal of Organic Chemistry; vol. 56; nb. 10; (1991); p. 3286 - 3294, View in Reaxys	
	NMR Spectroscopy (9)	
1 of 9	Description	Chemical shifts
	Nucleus	1H
	Solvents	chloroform-d1
	Frequency [MHz]	300
	Chernega, Alexander N.; Davies, Stephen G.; Hepworth, David; Kurosawa, Wataru; Roberts, Paul M.; Thomson, James E.; Goodwin, Christopher J. ; Organic Letters; vol. 11; nb. 15; (2009); p. 3254 - 3257, View in Reaxys	
2 of 9	Description	Spectrum
	Nucleus	1H
	Solvents	chloroform-d1
	Frequency [MHz]	400
	Chernega, Alexander N.; Davies, Stephen G.; Hepworth, David; Kurosawa, Wataru; Roberts, Paul M.; Thomson, James E.; Goodwin, Christopher J. ; Organic Letters; vol. 11; nb. 15; (2009); p. 3254 - 3257, View in Reaxys	
3 of 9	Description	Chemical shifts

	Nucleus	1H
	Solvents	CDCl3
	Frequency [MHz]	250
	Tessier, Arnaud; Pytkowicz, Julien; Brigaud, Thierry ; Angewandte Chemie, International Edition; vol. 45; nb. 22; (2006); p. 3677 - 3681; Angewandte Chemie; vol. 118; nb. 22; (2006); p. 3759 - 3763, View in Reaxys	
4 of 9	Description	Chemical shifts
	Nucleus	13C
	Solvents	CDCl3
	Frequency [MHz]	62.9
	Tessier, Arnaud; Pytkowicz, Julien; Brigaud, Thierry ; Angewandte Chemie, International Edition; vol. 45; nb. 22; (2006); p. 3677 - 3681; Angewandte Chemie; vol. 118; nb. 22; (2006); p. 3759 - 3763, View in Reaxys	
5 of 9	Description	Chemical shifts
	Nucleus	1H
	Solvents	CDCl3
	Frequency [MHz]	400
	Bull, Steven D.; Davies, Stephen G.; Nicholson, Rebecca L.; Sanganee, Hitesh J.; Smith, Andrew D. ; Organic and Biomolecular Chemistry; vol. 1; nb. 16; (2003); p. 2886 - 2899, View in Reaxys	
6 of 9	Nucleus	1H
	Coupling Nuclei	1H
	Solvents	CDCl3
	Frequency [MHz]	400
	Bull, Steven D.; Davies, Stephen G.; Nicholson, Rebecca L.; Sanganee, Hitesh J.; Smith, Andrew D. ; Organic and Biomolecular Chemistry; vol. 1; nb. 16; (2003); p. 2886 - 2899, View in Reaxys	
7 of 9	Description	Chemical shifts
	Nucleus	1H
	Solvents	CDCl3
		Rangaishenvi, Milind V.; Singaram, Bakthan; Brown, Herbert C. ; Journal of Organic Chemistry; vol. 56; nb. 10; (1991); p. 3286 - 3294, View in Reaxys
8 of 9	Description	Chemical shifts
	Nucleus	13C
	Solvents	CDCl3
		Rangaishenvi, Milind V.; Singaram, Bakthan; Brown, Herbert C. ; Journal of Organic Chemistry; vol. 56; nb. 10; (1991); p. 3286 - 3294, View in Reaxys
9 of 9	Description	Spin-spin coupling constants
	Solvents	CDCl3
	Comment	1H-1H
		Rangaishenvi, Milind V.; Singaram, Bakthan; Brown, Herbert C. ; Journal of Organic Chemistry; vol. 56; nb. 10; (1991); p. 3286 - 3294, View in Reaxys
IR Spectroscopy (1)		
Description	References	
Bands	Enders,D.; Eichenauer,H. ; Chemische Berichte; vol. 112; (1979); p. 2933 - 2960, View in Reaxys	



Chemical Name: (R)-2-methyl-3-phenylpropionaldehyde; (2R)-2-methyl-3-phenylpropan-1-al; (R)-2-methyldihydrocinnamaldehyde; (R)-2-methyl-3-phenylpropanal; (R)- α -methyl benzenepropanal; (R)-2-methyl-3-phenyl-propionaldehyde
Molecular Formula: C₁₀H₁₂O
CAS Registry Number: 5445-77-2; 42307-59-5; 63262-79-3; 78964-59-7
Molecular Weight: 148.205
Linear Structure Formula: HCOC₃H₆C₆H₅
Type of Substance: isocyclic
InChIKey: HEPHYCJJLAUKSB-SECBINFHSA-N
Note:

Substance Label (6)

Label	References
7af	Baeza, Alejandro; Najera, Carmen; Sansano, Jose M. ; European Journal of Organic Chemistry; nb. 7; (2007); p. 1101 - 1112, View in Reaxys
ent-30	Bull, Steven D.; Davies, Stephen G.; Nicholson, Rebecca L.; Sanganee, Hitesh J.; Smith, Andrew D. ; Organic and Biomolecular Chemistry; vol. 1; nb. 16; (2003); p. 2886 - 2899, View in Reaxys
6c	Tyrrell, Elizabeth; Skinner, George A.; Janes, John; Milsom, Greig ; Synlett; nb. 7; (2002); p. 1073 - 1076, View in Reaxys
44	Naito, Satoru; Escobar, Maya; Kym, Philip R.; Liras, Spiros; Martin, Stephen F. ; Journal of Organic Chemistry; vol. 67; nb. 12; (2002); p. 4200 - 4208, View in Reaxys
6	Kelly, Clare L.; Lawrie, Kenneth W. M.; Morgan, Paul; Willis, Christine L. ; Tetrahedron Letters; vol. 41; nb. 41; (2000); p. 8001 - 8005, View in Reaxys
(R)-15a	Bull, Steven D.; Davies, Stephen G.; Nicholson, Rebecca L.; Sanganee, Hitesh J.; Smith, Andrew D. ; Tetrahedron: Asymmetry; vol. 11; nb. 17; (2000); p. 3475 - 3480, View in Reaxys

Boiling Point (1)

Boiling Point [°C]	Pressure [Torr]	References
80 - 100	2	Davenport et al. ; Journal of the American Chemical Society; vol. 101; (1979); p. 5654,5658, View in Reaxys

Optical Rotatory Power (1)

1 of 1	Type	[alpha]
	Concentration	0.40 g/100ml
	Solvent	acetone
	Optical Rotatory Power [deg]	-4.75
	Wavelength [nm]	589
	Temperature [°C]	20
	Tanner, David; Birgersson, Carin; Gogoll, Adolf; Luthman, Kristina ; Tetrahedron; vol. 50; nb. 32; (1994); p. 9797 - 9824, View in Reaxys	

NMR Spectroscopy (8)

1 of 8	Description	Chemical shifts
	Nucleus	¹ H
	Solvents	CDCl ₃
	Frequency [MHz]	300
	Baeza, Alejandro; Najera, Carmen; Sansano, Jose M. ; European Journal of Organic Chemistry; nb. 7; (2007); p. 1101 - 1112, View in Reaxys	
2 of 8	Description	Chemical shifts
	Nucleus	¹ H
	Solvents	CDCl ₃
	Tanner, David; Birgersson, Carin; Gogoll, Adolf; Luthman, Kristina ; Tetrahedron; vol. 50; nb. 32; (1994); p. 9797 - 9824, View in Reaxys ; Oppolzer, Wolfgang; Darcel, Christophe; Rochet, Patrick; Rosset, Stephane; Brabander, Jef De ; Helvetica Chimica Acta; vol. 80; nb. 5; (1997); p. 1319 - 1337, View in Reaxys	

3 of 8	Description	Chemical shifts		
	Nucleus	13C		
	Solvents	CDCl3		
	Oppolzer, Wolfgang; Darcel, Christophe; Rochet, Patrick; Rosset, Stephane; Brabander, Jef De ; Helvetica Chimica Acta; vol. 80; nb. 5; (1997); p. 1319 - 1337, View in Reaxys ; Myers, Andrew G.; Yang, Bryant H.; Chen, Hou; McKinstry, Lydia; Kopecky, David J.; Gleason, James L. ; Journal of the American Chemical Society; vol. 119; nb. 28; (1997); p. 6496 - 6511, View in Reaxys			
4 of 8	Description	Chemical shifts		
	Nucleus	1H		
	Solvents	benzene-d6		
	Myers, Andrew G.; Yang, Bryant H.; Chen, Hou; McKinstry, Lydia; Kopecky, David J.; Gleason, James L. ; Journal of the American Chemical Society; vol. 119; nb. 28; (1997); p. 6496 - 6511, View in Reaxys			
5 of 8	Description	Spin-spin coupling constants		
	Solvents	CDCl3		
	Comment	1H-1H		
	Tanner, David; Birgersson, Carin; Gogoll, Adolf; Luthman, Kristina ; Tetrahedron; vol. 50; nb. 32; (1994); p. 9797 - 9824, View in Reaxys ; Oppolzer, Wolfgang; Darcel, Christophe; Rochet, Patrick; Rosset, Stephane; Brabander, Jef De ; Helvetica Chimica Acta; vol. 80; nb. 5; (1997); p. 1319 - 1337, View in Reaxys			
6 of 8	Description	Spin-spin coupling constants		
	Solvents	benzene-d6		
	Comment	1H-1H		
	Myers, Andrew G.; Yang, Bryant H.; Chen, Hou; McKinstry, Lydia; Kopecky, David J.; Gleason, James L. ; Journal of the American Chemical Society; vol. 119; nb. 28; (1997); p. 6496 - 6511, View in Reaxys			
7 of 8	Nucleus	1H		
	Solvents	C6D6		
	Frequency [MHz]	300		
	Original Text	1H NMR (300 MHz, C6D6) δ 9.29 (d, 1H, J=1.2 Hz), 6.8-7.12 (m, 5H), 2.72 (dd, 1H, J=13.2 Hz, 5.4 Hz), 2.0-2.2 (m, 2H), 0.69 (d, 3H, J=6.9 Hz);		
	Patent; California Institute of Technology ; US5488131; (1996); (A1) English, View in Reaxys			
8 of 8	Nucleus	13C		
	Solvents	CDCl3		
	Frequency [MHz]	75.5		
	Original Text	13C NMR (75.5 MHz, CDCl3) δ 204.3, 138.7, 128.9, 128.4, 126.3, 48.0, 36.5, 13.1		
	Patent; California Institute of Technology ; US5488131; (1996); (A1) English, View in Reaxys			
IR Spectroscopy (3)				
Description	Solvent	Original Text	Comment	References
Bands	neat (no solvent)		3026 - 1454 cm ^{**} (-1)	Oppolzer, Wolfgang; Darcel, Christophe; Rochet, Patrick; Rosset, Stephane; Brabander, Jef De ; Helvetica Chimica Acta; vol. 80; nb. 5; (1997); p. 1319 - 1337, View in Reaxys
		FTIR (neat film) cm-1 3028 (m), 2971 (m), 1932 (m), 2814 (w), 2716 (w), 1723 (s), 1496 (m), 1454 (m), 742 (m), 701 (s)		Patent; California Institute of Technology ; US5488131; (1996); (A1) English, View in Reaxys
Bands			1721 cm ^{**} (-1)	Tanner, David; Birgersson, Carin; Gogoll, Adolf; Luthman, Kristina ; Tetrahedron; vol. 50; nb. 32; (1994); p. 9797 - 9824, View in Reaxys

Mass Spectrometry (1)	
Description	References
spectrum	Oppolzer, Wolfgang; Darcel, Christophe; Rochet, Patrick; Rosset, Stephane; Brabander, Jef De; Helvetica Chimica Acta; vol. 80; nb. 5; (1997); p. 1319 - 1337, View in Reaxys