Butanoic acid, 3-methyl-, 2-phenylethyl ester

Other names:	Isovaleric acid, phenethyl ester «beta»-Phenylethyl isovalerate Phenethyl isovalerate 2-Phenylethyl 3-methylbutanoate Phenylethyl isovalerate 2-Phenylethyl 3-methylbutirate 2-Phenylethyl isopentanoate 2-phenylethyl isovalerate Phenyl ethyl 3-methyl-butanoate phenylethyl 3-methylbutyrate
Inchi:	InChI=1S/C13H18O2/c1-11(2)10-13(14)15-9-8-12-6-4-3-5-7-12/h3-7,11H,8-10H2,1-2H3
InchiKey:	JIMGVOCOYZFDKB-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CC(C)CC(=O)OCCc1ccccc1
Mol. weight [g/mol]:	206.28
CAS:	140-26-1

Physical Properties

Property code	Value	Unit	Source
gf	-65.37	kJ/mol	Joback Method
hf	-325.20	kJ/mol	Joback Method
hfus	22.73	kJ/mol	Joback Method
hvap	55.58	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.818		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	1488.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1466.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1494.70		NIST Webbook

rinpol	1499.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1457.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1490.00		NIST Webbook
ripol	1992.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	1983.00		NIST Webbook
ripol	1980.00		NIST Webbook
ripol	1986.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1927.00		NIST Webbook
tb	599.37	K	Joback Method
tc	806.35	K	Joback Method
tf	319.85	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.71	J/mol×K	599.37	Joback Method
cpg	459.89	J/mol×K	633.87	Joback Method
cpg	475.13	J/mol×K	668.36	Joback Method
cpg	489.48	J/mol×K	702.86	Joback Method
cpg	502.95	J/mol×K	737.36	Joback Method
cpg	515.57	J/mol×K	771.85	Joback Method
cpg	527.37	J/mol×K	806.35	Joback Method
dvisc	0.0027865	Pa×s	319.85	Joback Method
dvisc	0.0012714	Pa×s	366.44	Joback Method
dvisc	0.0006925	Pa×s	413.02	Joback Method
dvisc	0.0004266	Pa×s	459.61	Joback Method
dvisc	0.0002873	Pa×s	506.20	Joback Method
dvisc	0.0002068	Pa×s	552.78	Joback Method
dvisc	0.0001567	Pa×s	599.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C140261&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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