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

Other names:	Phenethyl 2-methylbutyrate
	2-Phenylethyl 2-methylbutanoate
	2-Phenylethyl 2-methylbutyrate
	Phenethyl 2-methylbutanoate
	Phenylethyl 2-methylbutanoate
	FEMA 3632
	«beta»-Phenethyl «alpha»-methylbutanoate
	Butyric acid, 2-methyl-, phenethyl ester
	Phenylethyl 2-methylbutyrate
Inchi:	InChI=1S/C13H18O2/c1-3-11(2)13(14)15-10-9-12-7-5-4-6-8-12/h4-8,11H,3,9-10H2,1-2H
InchiKey:	KVKKTLBBYFABAZ-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CCC(C)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	206.28
CAS:	24817-51-4

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	1466.00		NIST Webbook
rinpol	1491.30		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1460.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1472.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	1945.00		NIST Webbook

ripol	1988.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1950.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	1968.00		NIST Webbook
ripol	1988.00		NIST Webbook
ripol	1964.00		NIST Webbook
ripol	1950.00		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	515.57	J/mol×K	771.85	Joback Method
cpg	502.95	J/mol×K	737.36	Joback Method
cpg	489.48	J/mol×K	702.86	Joback Method
cpg	475.13	J/mol×K	668.36	Joback Method
cpg	459.89	J/mol×K	633.87	Joback Method
cpg	527.37	J/mol×K	806.35	Joback Method
dvisc	0.0001567	Pa×s	599.37	Joback Method
dvisc	0.0002068	Pa×s	552.78	Joback Method
dvisc	0.0002873	Pa×s	506.20	Joback Method
dvisc	0.0004266	Pa×s	459.61	Joback Method
dvisc	0.0006925	Pa×s	413.02	Joback Method
dvisc	0.0012714	Pa×s	366.44	Joback Method
dvisc	0.0027865	Pa×s	319.85	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C24817514&Units=SI

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