Propanoic acid, 2,2-dimethyl-, 2-phenylethyl ester

Other names:	Phenethyl pivalate
	2,2-Dimethylpropionic acid, 2-phenylethyl ester
	Pivalic acid, 2-phenylethyl ester
	Phenylethyl pivalate
	Pivarose
	Centifolyl
	2,2-Dimethylpropanoic acid, 2-phenylethyl ester
Inchi:	InChI=1S/C13H18O2/c1-13(2,3)12(14)15-10-9-11-7-5-4-6-8-11/h4-8H,9-10H2,1-3H3
InchiKey:	DPVYDTACPLLHCF-UHFFFAOYSA-N
Formula:	C13H18O2
SMILES:	CC(C)(C)C(=O)OCCc1ccccc1
Mol. weight [g/mol]:	206.28
CAS:	67662-96-8

Physical Properties

Property code	Value	Unit	Source
gf	-60.09	kJ/mol	Joback Method
hf	-328.67	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	54.67	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.818		Crippen Method
mcvol	177.710	ml/mol	McGowan Method
pc	2333.78	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1801.00		NIST Webbook
ripol	1832.00		NIST Webbook
tb	596.58	K	Joback Method
tc	811.41	K	Joback Method
tf	337.27	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.48	J/mol×K	596.58	Joback Method
cpg	463.14	J/mol×K	632.38	Joback Method
cpg	478.72	J/mol×K	668.19	Joback Method
cpg	493.27	J/mol×K	703.99	Joback Method
cpg	506.83	J/mol×K	739.80	Joback Method
cpg	519.47	J/mol×K	775.60	Joback Method
cpg	531.22	J/mol×K	811.41	Joback Method
dvisc	0.0024771	Pa×s	337.27	Joback Method
dvisc	0.0011900	Pa×s	380.49	Joback Method
dvisc	0.0006639	Pa×s	423.71	Joback Method
dvisc	0.0004127	Pa×s	466.92	Joback Method
dvisc	0.0002780	Pa×s	510.14	Joback Method
dvisc	0.0001992	Pa×s	553.36	Joback Method
dvisc	0.0001498	Pa×s	596.58	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C67662968&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

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

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