Butanoic acid, 3-methyl-, 5-methyl-2-(1-methylethyl)cyclohexyl ester, (1«alpha»,2«beta»,5«alpha»)-

Other names: (1«alpha»,2«beta»,5«alpha»)-3-Methylbutanoic acid 5-methyl-2-(1-methylethyl)cyclohexyl ester
Menthyl valerate
Validol

Inchi: InChI=1S/C15H28O2/c1-5-6-7-15(16)17-14-10-12(4)8-9-13(14)11(2)3/h11-14H,5-10H2,1

InchiKey: LCJPVSLESAPYMK-UHFFFAOYSA-N

Formula: C15H28O2

SMILES: CCCCC(=O)OC1CC(C)CCC1C(C)C

Mol. weight [g/mol]: 240.38

CAS: 89-47-4

Physical Properties

Property code	Value	Unit	Source
gf	-151.91	kJ/mol	Joback Method
hf	-589.37	kJ/mol	Joback Method
hfus	27.85	kJ/mol	Joback Method
hvap	57.56	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.181		Crippen Method
mcvol	218.790	ml/mol	McGowan Method
pc	1645.76	kPa	Joback Method
tb	628.66	K	Joback Method
tc	823.75	K	Joback Method
tf	314.87	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.44	J/mol×K	628.66	Joback Method
cpg	638.98	J/mol×K	661.18	Joback Method
cpg	659.41	J/mol×K	693.69	Joback Method
cpg	678.75	J/mol×K	726.21	Joback Method
cpg	697.00	J/mol×K	758.72	Joback Method
cpg	714.18	J/mol×K	791.24	Joback Method

cpg	730.29	J/mol×K	823.75	Joback Method
dvisc	0.0030275	Pa×s	314.87	Joback Method
dvisc	0.0013669	Pa×s	367.17	Joback Method
dvisc	0.0007525	Pa×s	419.47	Joback Method
dvisc	0.0004729	Pa×s	471.76	Joback Method
dvisc	0.0003260	Pa×s	524.06	Joback Method
dvisc	0.0002405	Pa×s	576.36	Joback Method
dvisc	0.0001866	Pa×s	628.66	Joback Method

Sources

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=C89474&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume