3-Cyclohexene-1-methanol, «alpha»,«alpha»,4-trimethyl-, propanoate

Other names: «alpha»-Terpinyl propionate
4-Terpinenyl ester of propanoic acid
«alpha»-Terpinyl ester of propanoic acid
Terpinyl n-propionate
Terpinyl propionate
Terpenyl propionate
p-menth-1-en-8-yl propionate

Inchi: InChI=1S/C13H22O2/c1-5-12(14)15-13(3,4)11-8-6-10(2)7-9-11/h6,11H,5,7-9H2,1-4H3

InchiKey: CMKQOKAXUWQAHG-UHFFFAOYSA-N

Formula: C13H22O2

SMILES: CCC(=O)OC(C)(C)C1CC=C(C)CC1

Mol. weight [g/mol]: 210.31

CAS: 80-27-3

Physical Properties

Property code	Value	Unit	Source
gf	-127.72	kJ/mol	Joback Method
hf	-464.57	kJ/mol	Joback Method
hfus	17.47	kJ/mol	Joback Method
hvap	53.77	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.465		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	1426.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1431.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1398.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1747.00		NIST Webbook
ripol	1747.00		NIST Webbook
tb	593.59	K	Joback Method
tc	804.49	K	Joback Method

tf	331.51	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.08	J/mol×K	593.59	Joback Method
cpg	508.39	J/mol×K	628.74	Joback Method
cpg	526.55	J/mol×K	663.89	Joback Method
cpg	543.61	J/mol×K	699.04	Joback Method
cpg	559.60	J/mol×K	734.19	Joback Method
cpg	574.56	J/mol×K	769.34	Joback Method
cpg	588.53	J/mol×K	804.49	Joback Method
dvisc	0.0027570	Pa×s	331.51	Joback Method
dvisc	0.0013092	Pa×s	375.19	Joback Method
dvisc	0.0007262	Pa×s	418.87	Joback Method
dvisc	0.0004502	Pa×s	462.55	Joback Method
dvisc	0.0003031	Pa×s	506.23	Joback Method
dvisc	0.0002173	Pa×s	549.91	Joback Method
dvisc	0.0001636	Pa×s	593.59	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=C80273&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