Propanoic acid, 3-hydroxy-2-methyl, 2,4,4-trimethylpentyl ester

Other names: propionic acid, -3-hydroxy-2-methyl-, 2,4,4-trimethylpentyl ester
Inchi: InChI=1S/C12H24O3/c1-9(6-12(3,4)5)8-15-11(14)10(2)7-13/h9-10,13H,6-8H2,1-5H3
InchiKey: UWYBMAMAOBQGNK-UHFFFAOYSA-N
Formula: C12H24O3
SMILES: CC(COC(=O)C(C)CO)CC(C)(C)C
Mol. weight [g/mol]: 216.32

Physical Properties

Property code	Value	Unit	Source
gf	-322.62	kJ/mol	Joback Method
hf	-707.35	kJ/mol	Joback Method
hfus	19.25	kJ/mol	Joback Method
hvap	66.07	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.230		Crippen Method
mcvol	193.250	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	1387.00		NIST Webbook
tb	638.32	K	Joback Method
tc	816.40	K	Joback Method
tf	330.40	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.96	J/mol×K	638.32	Joback Method
cpg	548.50	J/mol×K	668.00	Joback Method
cpg	562.30	J/mol×K	697.68	Joback Method
cpg	575.41	J/mol×K	727.36	Joback Method
cpg	587.84	J/mol×K	757.04	Joback Method
cpg	599.62	J/mol×K	786.72	Joback Method
cpg	610.77	J/mol×K	816.40	Joback Method
dvisc	0.0111802	Pa×s	330.40	Joback Method

dvisc	0.0023392	Pa×s	381.72	Joback Method
dvisc	0.0007091	Pa×s	433.04	Joback Method
dvisc	0.0002768	Pa×s	484.36	Joback Method
dvisc	0.0001294	Pa×s	535.68	Joback Method
dvisc	0.0000691	Pa×s	587.00	Joback Method
dvisc	0.0000408	Pa×s	638.32	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=R288736&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume