propionic acid, 2-methyl-2,2-dimethyl-1-(2-hydroxy-1-methylethyl propyl ester

Inchi: InChI=1S/C14H28O3/c1-9(2)11(8-15)12(14(5,6)7)17-13(16)10(3)4/h9-12,15H,8H2,1-7H3

InchiKey: TUFUAULJMNPJTI-UHFFFAOYSA-N

Formula: C14H28O3

SMILES: CC(C)C(=O)OC(C(CO)C(C)C)C(C)(C)C

Mol. weight [g/mol]: 244.37

Physical Properties

Property code	Value	Unit	Source
gf	-310.66	kJ/mol	Joback Method
hf	-759.19	kJ/mol	Joback Method
hfus	17.39	kJ/mol	Joback Method
hvap	69.75	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.865		Crippen Method
mcvol	221.430	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	1389.00		NIST Webbook
rinpol	1389.00		NIST Webbook
tb	683.20	K	Joback Method
tc	864.80	K	Joback Method
tf	322.94	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.87	J/mol×K	683.20	Joback Method
cpg	713.57	J/mol×K	834.53	Joback Method
cpg	700.79	J/mol×K	804.27	Joback Method
cpg	687.25	J/mol×K	774.00	Joback Method
cpg	672.94	J/mol×K	743.73	Joback Method
cpg	657.83	J/mol×K	713.47	Joback Method
cpg	725.62	J/mol×K	864.80	Joback Method
dvisc	0.0000235	Pa×s	683.20	Joback Method

dvisc	0.0000419	Pa×s	623.16	Joback Method
dvisc	0.0000846	Pa×s	563.11	Joback Method
dvisc	0.0002021	Pa×s	503.07	Joback Method
dvisc	0.0006113	Pa×s	443.03	Joback Method
dvisc	0.0026162	Pa×s	382.98	Joback Method
dvisc	0.0192254	Pa×s	322.94	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=R519852&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