Diglycolic acid, isobutyl 2-methylpentyl ester

Inchi: InChI=1S/C14H26O5/c1-5-6-12(4)8-19-14(16)10-17-9-13(15)18-7-11(2)3/h11-12H,5-10H
InchiKey: OYZRBLGGNFRDSJ-UHFFFAOYSA-N
Formula: C14H26O5
SMILES: CCCC(C)COC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]: 274.35

Physical Properties

Property code	Value	Unit	Source
gf	-510.72	kJ/mol	Joback Method
hf	-964.67	kJ/mol	Joback Method
hfus	31.73	kJ/mol	Joback Method
hvap	66.70	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	2.182		Crippen Method
mcvol	228.870	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2177.00		NIST Webbook
rinpol	2177.00		NIST Webbook
tb	693.84	K	Joback Method
tc	874.69	K	Joback Method
tf	384.09	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.96	J/mol×K	693.84	Joback Method
cpg	667.87	J/mol×K	723.98	Joback Method
cpg	682.99	J/mol×K	754.12	Joback Method
cpg	697.31	J/mol×K	784.26	Joback Method
cpg	710.83	J/mol×K	814.40	Joback Method
cpg	723.55	J/mol×K	844.55	Joback Method
cpg	735.46	J/mol×K	874.69	Joback Method
dvisc	0.0015512	Pa×s	384.09	Joback Method

dvisc	0.0007036	Pa×s	435.72	Joback Method
dvisc	0.0003773	Pa×s	487.34	Joback Method
dvisc	0.0002280	Pa×s	538.97	Joback Method
dvisc	0.0001504	Pa×s	590.59	Joback Method
dvisc	0.0001061	Pa×s	642.22	Joback Method
dvisc	0.0000789	Pa×s	693.84	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=U381794&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