Diglycolic acid, isohexyl 2-methylpentyl ester

Inchi: InChI=1S/C16H30O5/c1-5-7-14(4)10-21-16(18)12-19-11-15(17)20-9-6-8-13(2)3/h13-14H
InchiKey: YXQJONITTBYSHW-UHFFFAOYSA-N
Formula: C16H30O5
SMILES: CCCC(C)COC(=O)COCC(=O)OCCCC(C)C
Mol. weight [g/mol]: 302.41

Physical Properties

Property code	Value	Unit	Source
gf	-493.88	kJ/mol	Joback Method
hf	-1005.95	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.962		Crippen Method
mcvol	257.050	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	2451.00		NIST Webbook
rinpol	2451.00		NIST Webbook
tb	739.60	K	Joback Method
tc	920.56	K	Joback Method
tf	406.63	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.62	J/mol×K	739.60	Joback Method
cpg	781.34	J/mol×K	769.76	Joback Method
cpg	797.17	J/mol×K	799.92	Joback Method
cpg	812.09	J/mol×K	830.08	Joback Method
cpg	826.12	J/mol×K	860.24	Joback Method
cpg	839.25	J/mol×K	890.40	Joback Method
cpg	851.49	J/mol×K	920.56	Joback Method
dvisc	0.0012606	Pa×s	406.63	Joback Method

dvisc	0.0005594	Pa×s	462.12	Joback Method
dvisc	0.0002955	Pa×s	517.62	Joback Method
dvisc	0.0001766	Pa×s	573.12	Joback Method
dvisc	0.0001156	Pa×s	628.61	Joback Method
dvisc	0.0000810	Pa×s	684.11	Joback Method
dvisc	0.0000599	Pa×s	739.60	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=U381797&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume