Diglycolic acid, isohexyl 3-methylpent-2-yl ester

Inchi: InChI=1S/C16H30O5/c1-6-13(4)14(5)21-16(18)11-19-10-15(17)20-9-7-8-12(2)3/h12-14H

InchiKey: IRSWFJQPQMUMLQ-UHFFFAOYSA-N

Formula: C16H30O5

SMILES: CCC(C)C(C)OC(=O)COCC(=O)OCCCC(C)C

Mol. weight [g/mol]: 302.41

Physical Properties

Property code	Value	Unit	Source
gf	-496.32	kJ/mol	Joback Method
hf	-1011.23	kJ/mol	Joback Method
hfus	33.39	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.960		Crippen Method
mcvol	257.050	ml/mol	McGowan Method
pc	1418.64	kPa	Joback Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	739.16	K	Joback Method
tc	922.02	K	Joback Method
tf	391.63	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.12	J/mol×K	739.16	Joback Method
cpg	782.03	J/mol×K	769.64	Joback Method
cpg	798.01	J/mol×K	800.11	Joback Method
cpg	813.08	J/mol×K	830.59	Joback Method
cpg	827.22	J/mol×K	861.06	Joback Method
cpg	840.43	J/mol×K	891.54	Joback Method
cpg	852.72	J/mol×K	922.02	Joback Method
dvisc	0.0015736	Pa×s	391.63	Joback Method

dvisc	0.0006286	Pa×s	449.55	Joback Method
dvisc	0.0003096	Pa×s	507.47	Joback Method
dvisc	0.0001763	Pa×s	565.39	Joback Method
dvisc	0.0001115	Pa×s	623.32	Joback Method
dvisc	0.0000762	Pa×s	681.24	Joback Method
dvisc	0.0000553	Pa×s	739.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381873&Units=SI
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

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