Diglycolic acid, isohexyl neopentyl ester

Inchi: InChI=1S/C15H28O5/c1-12(2)7-6-8-19-13(16)9-18-10-14(17)20-11-15(3,4)5/h12H,6-11H
InchiKey: FKOSFJAESXOTJC-UHFFFAOYSA-N
Formula: C15H28O5
SMILES: CC(C)CCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 288.38

Physical Properties

Property code	Value	Unit	Source
gf	-497.02	kJ/mol	Joback Method
hf	-988.78	kJ/mol	Joback Method
hfus	30.43	kJ/mol	Joback Method
hvap	68.02	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.572		Crippen Method
mcvol	242.960	ml/mol	McGowan Method
pc	1530.66	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	713.93	K	Joback Method
tc	898.50	K	Joback Method
tf	412.78	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.41	J/mol×K	713.93	Joback Method
cpg	725.84	J/mol×K	744.69	Joback Method
cpg	741.38	J/mol×K	775.45	Joback Method
cpg	756.04	J/mol×K	806.22	Joback Method
cpg	769.83	J/mol×K	836.98	Joback Method
cpg	782.75	J/mol×K	867.74	Joback Method
cpg	794.83	J/mol×K	898.50	Joback Method
dvisc	0.0011564	Pa×s	412.78	Joback Method

dvisc	0.0005456	Pa×s	462.97	Joback Method
dvisc	0.0002982	Pa×s	513.16	Joback Method
dvisc	0.0001815	Pa×s	563.36	Joback Method
dvisc	0.0001198	Pa×s	613.55	Joback Method
dvisc	0.0000842	Pa×s	663.74	Joback Method
dvisc	0.0000622	Pa×s	713.93	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=U381918&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