

Diglycolic acid, hexyl isobutyl ester

Inchi:	InChI=1S/C14H26O5/c1-4-5-6-7-8-18-13(15)10-17-11-14(16)19-9-12(2)3/h12H,4-11H2,1
InchiKey:	UCXRPGWEAKGNPH-UHFFFAOYSA-N
Formula:	C14H26O5
SMILES:	CCCCCOC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]:	274.35

Physical Properties

Property code	Value	Unit	Source
gf	-508.28	kJ/mol	Joback Method
hf	-959.39	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.326		Crippen Method
mcvol	228.870	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpola	2201.00		NIST Webbook
rinpola	2201.00		NIST Webbook
tb	694.28	K	Joback Method
tc	872.83	K	Joback Method
tf	399.09	K	Joback Method
vc	0.879	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.48	J/molxK	694.28	Joback Method
cpg	667.16	J/molxK	724.04	Joback Method
cpg	682.08	J/molxK	753.80	Joback Method
cpg	696.23	J/molxK	783.56	Joback Method
cpg	709.61	J/molxK	813.32	Joback Method
cpg	722.22	J/molxK	843.08	Joback Method
cpg	734.04	J/molxK	872.83	Joback Method
dvisc	0.0012554	Paxs	399.09	Joback Method

dvisc	0.0006269	Paxs	448.29	Joback Method
dvisc	0.0003592	Paxs	497.49	Joback Method
dvisc	0.0002275	Paxs	546.68	Joback Method
dvisc	0.0001553	Paxs	595.88	Joback Method
dvisc	0.0001124	Paxs	645.08	Joback Method
dvisc	0.0000852	Paxs	694.28	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U382129&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

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