

Diglycolic acid, hexyl neopentyl ester

Inchi:	InChI=1S/C15H28O5/c1-5-6-7-8-9-19-13(16)10-18-11-14(17)20-12-15(2,3)4/h5-12H2,1-4
InchiKey:	RWJVCRSCIPIEGQ-UHFFFAOYSA-N
Formula:	C15H28O5
SMILES:	CCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	288.38

Physical Properties

Property code	Value	Unit	Source
gf	-494.58	kJ/mol	Joback Method
hf	-983.50	kJ/mol	Joback Method
hfus	33.95	kJ/mol	Joback Method
hvap	68.41	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.716		Crippen Method
mvol	242.960	ml/mol	McGowan Method
pc	1521.12	kPa	Joback Method
rinpol	2254.00		NIST Webbook
rinpol	2254.00		NIST Webbook
tb	714.37	K	Joback Method
tc	896.66	K	Joback Method
tf	427.78	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.91	J/molxK	714.37	Joback Method
cpg	725.12	J/molxK	744.75	Joback Method
cpg	740.47	J/molxK	775.13	Joback Method
cpg	754.97	J/molxK	805.52	Joback Method
cpg	768.62	J/molxK	835.90	Joback Method
cpg	781.44	J/molxK	866.28	Joback Method
cpg	793.43	J/molxK	896.66	Joback Method
dvisc	0.0009493	Paxs	427.78	Joback Method

dvisc	0.0004894	Paxs	475.54	Joback Method
dvisc	0.0002847	Paxs	523.31	Joback Method
dvisc	0.0001813	Paxs	571.08	Joback Method
dvisc	0.0001238	Paxs	618.84	Joback Method
dvisc	0.0000893	Paxs	666.61	Joback Method
dvisc	0.0000673	Paxs	714.37	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=U381919&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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