

Diglycolic acid, isohexyl 3-methylbutyl ester

Inchi:	InChI=1S/C15H28O5/c1-12(2)6-5-8-19-14(16)10-18-11-15(17)20-9-7-13(3)4/h12-13H,5-
InchiKey:	YANGXWXQQZWAPO-UHFFFAOYSA-N
Formula:	C15H28O5
SMILES:	CC(C)CCCOC(=O)COCC(=O)OCCC(C)C
Mol. weight [g/mol]:	288.38

Physical Properties

Property code	Value	Unit	Source
gf	-502.30	kJ/mol	Joback Method
hf	-985.31	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	68.93	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.572		Crippen Method
mvol	242.960	ml/mol	McGowan Method
pc	1517.57	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	716.72	K	Joback Method
tc	897.37	K	Joback Method
tf	395.36	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.73	J/molxK	716.72	Joback Method
cpg	780.93	J/molxK	867.26	Joback Method
cpg	767.99	J/molxK	837.15	Joback Method
cpg	754.19	J/molxK	807.05	Joback Method
cpg	739.55	J/molxK	776.94	Joback Method
cpg	724.06	J/molxK	746.83	Joback Method
cpg	793.03	J/molxK	897.37	Joback Method
dvisc	0.0000689	Paxs	716.72	Joback Method

dvisc	0.0000929	Paxs	663.16	Joback Method
dvisc	0.0001321	Paxs	609.60	Joback Method
dvisc	0.0002010	Paxs	556.04	Joback Method
dvisc	0.0003346	Paxs	502.48	Joback Method
dvisc	0.0006288	Paxs	448.92	Joback Method
dvisc	0.0014019	Paxs	395.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382271&Units=SI
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

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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