

Diglycolic acid, neopentyl nonyl ester

Inchi:	InChI=1S/C18H34O5/c1-5-6-7-8-9-10-11-12-22-16(19)13-21-14-17(20)23-15-18(2,3)4/h5
InchiKey:	HNXVKDWSMQLAPG-UHFFFAOYSA-N
Formula:	C18H34O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	330.46

Physical Properties

Property code	Value	Unit	Source
gf	-469.32	kJ/mol	Joback Method
hf	-1045.42	kJ/mol	Joback Method
hfus	41.72	kJ/mol	Joback Method
hvap	75.09	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.886		Crippen Method
mvol	285.230	ml/mol	McGowan Method
pc	1229.42	kPa	Joback Method
rinpol	2625.00		NIST Webbook
rinpol	2625.00		NIST Webbook
tb	783.01	K	Joback Method
tc	967.20	K	Joback Method
tf	461.59	K	Joback Method
vc	1.099	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.82	J/molxK	783.01	Joback Method
cpg	899.09	J/molxK	813.71	Joback Method
cpg	915.35	J/molxK	844.41	Joback Method
cpg	930.63	J/molxK	875.10	Joback Method
cpg	944.94	J/molxK	905.80	Joback Method
cpg	958.30	J/molxK	936.50	Joback Method
cpg	970.72	J/molxK	967.20	Joback Method
dvisc	0.0006811	Paxs	461.59	Joback Method

dvisc	0.0003384	Paxs	515.16	Joback Method
dvisc	0.0001918	Paxs	568.73	Joback Method
dvisc	0.0001199	Paxs	622.30	Joback Method
dvisc	0.0000808	Paxs	675.87	Joback Method
dvisc	0.0000576	Paxs	729.44	Joback Method
dvisc	0.0000431	Paxs	783.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381921&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	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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