

Diglycolic acid, neopentyl pentyl ester

Inchi:	InChI=1S/C14H26O5/c1-5-6-7-8-18-12(15)9-17-10-13(16)19-11-14(2,3)4/h5-11H2,1-4H3
InchiKey:	IMKYHWXLGSKCRH-UHFFFAOYSA-N
Formula:	C14H26O5
SMILES:	CCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	274.35

Physical Properties

Property code	Value	Unit	Source
gf	-503.00	kJ/mol	Joback Method
hf	-962.86	kJ/mol	Joback Method
hfus	31.36	kJ/mol	Joback Method
hvap	66.18	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	2.326		Crippen Method
mvol	228.870	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
rinpol	2133.00		NIST Webbook
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tb	691.49	K	Joback Method
tc	874.22	K	Joback Method
tf	416.51	K	Joback Method
vc	0.875	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.43	J/molxK	691.49	Joback Method
cpg	669.24	J/molxK	721.94	Joback Method
cpg	684.23	J/molxK	752.40	Joback Method
cpg	698.40	J/molxK	782.85	Joback Method
cpg	711.78	J/molxK	813.31	Joback Method
cpg	724.35	J/molxK	843.76	Joback Method
cpg	736.14	J/molxK	874.22	Joback Method
dvisc	0.0010508	Paxs	416.51	Joback Method

dvisc	0.0005490	Paxs	462.34	Joback Method
dvisc	0.0003225	Paxs	508.17	Joback Method
dvisc	0.0002068	Paxs	554.00	Joback Method
dvisc	0.0001420	Paxs	599.83	Joback Method
dvisc	0.0001028	Paxs	645.66	Joback Method
dvisc	0.0000777	Paxs	691.49	Joback Method

Sources

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=U381917&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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