

Diglycolic acid, ethyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C14H26O5/c1-6-18-12(15)9-17-10-13(16)19-8-11(2)7-14(3,4)5/h11H,6-10H2,1
InchiKey:	PIWQMEWLHIBKNH-UHFFFAOYSA-N
Formula:	C14H26O5
SMILES:	CCOC(=O)COCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	274.35

Physical Properties

Property code	Value	Unit	Source
gf	-505.44	kJ/mol	Joback Method
hf	-968.14	kJ/mol	Joback Method
hfus	27.84	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	2.182		Crippen Method
mvol	228.870	ml/mol	McGowan Method
pc	1652.46	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	691.05	K	Joback Method
tc	876.32	K	Joback Method
tf	401.51	K	Joback Method
vc	0.869	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.91	J/molxK	691.05	Joback Method
cpg	669.96	J/molxK	721.93	Joback Method
cpg	685.17	J/molxK	752.81	Joback Method
cpg	699.53	J/molxK	783.68	Joback Method
cpg	713.06	J/molxK	814.56	Joback Method
cpg	725.75	J/molxK	845.44	Joback Method
cpg	737.63	J/molxK	876.32	Joback Method
dvisc	0.0012897	Paxs	401.51	Joback Method

dvisc	0.0006159	Paxs	449.77	Joback Method
dvisc	0.0003394	Paxs	498.02	Joback Method
dvisc	0.0002078	Paxs	546.28	Joback Method
dvisc	0.0001378	Paxs	594.54	Joback Method
dvisc	0.0000972	Paxs	642.79	Joback Method
dvisc	0.0000720	Paxs	691.05	Joback Method

Sources

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=U382035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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