

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

Inchi:	InChI=1S/C27H52O5/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-19-31-25(28)22-30-23-26(
InchiKey:	JOKDPBYKKFGXDL-UHFFFAOYSA-N
Formula:	C27H52O5
SMILES:	CCCCCCCCCCCCCCCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	456.70

Physical Properties

Property code	Value	Unit	Source
gf	-395.98	kJ/mol	Joback Method
hf	-1236.46	kJ/mol	Joback Method
hfus	61.51	kJ/mol	Joback Method
hvap	94.73	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	7.253		Crippen Method
mcvol	412.040	ml/mol	McGowan Method
pc	727.31	kPa	Joback Method
rinsol	3658.00		NIST Webbook
tb	988.49	K	Joback Method
tc	1219.20	K	Joback Method
tf	548.02	K	Joback Method
vc	1.597	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1441.38	J/molxK	988.49	Joback Method
cpg	1462.25	J/molxK	1026.94	Joback Method
cpg	1481.25	J/molxK	1065.39	Joback Method
cpg	1498.43	J/molxK	1103.85	Joback Method
cpg	1513.86	J/molxK	1142.30	Joback Method
cpg	1527.61	J/molxK	1180.75	Joback Method
cpg	1539.76	J/molxK	1219.20	Joback Method
dvisc	0.0002391	Paxs	548.02	Joback Method
dvisc	0.0001012	Paxs	621.43	Joback Method

dvisc	0.0000513	Paxs	694.84	Joback Method
dvisc	0.0000297	Paxs	768.25	Joback Method
dvisc	0.0000189	Paxs	841.67	Joback Method
dvisc	0.0000129	Paxs	915.08	Joback Method
dvisc	0.0000093	Paxs	988.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382050&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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