Diglycolic acid, 2-pentyl pentyl ester

Inchi: InChI=1S/C14H26O5/c1-4-6-7-9-18-13(15)10-17-11-14(16)19-12(3)8-5-2/h12H,4-11H2,1
InchiKey: UKCDAODJCNZXKO-UHFFFAOYSA-N
Formula: C14H26O5
SMILES: CCCCCOC(=O)COCC(=O)OC(C)CCC
Mol. weight [g/mol]: 274.35

Physical Properties

Property code	Value	Unit	Source
gf	-508.28	kJ/mol	Joback Method
hf	-959.39	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	67.09	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.468		Crippen Method
mcvol	228.870	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2162.00		NIST Webbook
rinpol	2162.00		NIST Webbook
tb	694.28	K	Joback Method
tc	872.83	K	Joback Method
tf	399.09	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.48	J/mol×K	694.28	Joback Method
cpg	667.16	J/mol×K	724.04	Joback Method
cpg	682.08	J/mol×K	753.80	Joback Method
cpg	696.23	J/mol×K	783.56	Joback Method
cpg	709.61	J/mol×K	813.32	Joback Method
cpg	722.22	J/mol×K	843.08	Joback Method
cpg	734.04	J/mol×K	872.83	Joback Method
dvisc	0.0012554	Pa×s	399.09	Joback Method

dvisc	0.0006269	Pa×s	448.29	Joback Method
dvisc	0.0003592	Pa×s	497.49	Joback Method
dvisc	0.0002275	Pa×s	546.68	Joback Method
dvisc	0.0001553	Pa×s	595.88	Joback Method
dvisc	0.0001124	Pa×s	645.08	Joback Method
dvisc	0.0000852	Pa×s	694.28	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U382335&Units=SI

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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