Diglycolic acid, heptyl 2-pentyl ester

Inchi: InChI=1S/C16H30O5/c1-4-6-7-8-9-11-20-15(17)12-19-13-16(18)21-14(3)10-5-2/h14H,4-1
InchiKey: PIOMNSICODCCCY-UHFFFAOYSA-N
Formula: C16H30O5
SMILES: CCCCCCCOC(=O)COCC(=O)OC(C)CCC
Mol. weight [g/mol]: 302.41

Physical Properties

Property code	Value	Unit	Source
gf	-491.44	kJ/mol	Joback Method
hf	-1000.67	kJ/mol	Joback Method
hfus	40.44	kJ/mol	Joback Method
hvap	71.54	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.248		Crippen Method
mcvol	257.050	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2413.00		NIST Webbook
rinpol	2413.00		NIST Webbook
tb	740.04	K	Joback Method
tc	919.24	K	Joback Method
tf	421.63	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.13	J/mol×K	740.04	Joback Method
cpg	780.67	J/mol×K	769.91	Joback Method
cpg	796.34	J/mol×K	799.77	Joback Method
cpg	811.14	J/mol×K	829.64	Joback Method
cpg	825.07	J/mol×K	859.51	Joback Method
cpg	838.12	J/mol×K	889.37	Joback Method
cpg	850.30	J/mol×K	919.24	Joback Method
dvisc	0.0010358	Pa×s	421.63	Joback Method

dvisc	0.0005045	Pa×s	474.70	Joback Method
dvisc	0.0002839	Pa×s	527.77	Joback Method
dvisc	0.0001775	Pa×s	580.84	Joback Method
dvisc	0.0001200	Pa×s	633.90	Joback Method
dvisc	0.0000862	Pa×s	686.97	Joback Method
dvisc	0.0000650	Pa×s	740.04	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=U382338&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