Diglycolic acid, heptyl undecyl ester

Inchi: InChI=1S/C22H42O5/c1-3-5-7-9-10-11-12-14-16-18-27-22(24)20-25-19-21(23)26-17-15-
InchiKey: NZKNFHUCOQTSQD-UHFFFAOYSA-N
Formula: C22H42O5
SMILES: CCCCCCCCCCCOC(=O)COCC(=O)OCCCCCCC
Mol. weight [g/mol]: 386.57

Physical Properties

Property code	Value	Unit	Source
gf	-438.48	kJ/mol	Joback Method
hf	-1119.23	kJ/mol	Joback Method
hfus	59.50	kJ/mol	Joback Method
hvap	85.29	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	5.591		Crippen Method
mcvol	341.590	ml/mol	McGowan Method
pc	943.84	kPa	Joback Method
rinpol	3246.00		NIST Webbook
rinpol	3246.00		NIST Webbook
tb	877.76	K	Joback Method
tc	1074.82	K	Joback Method
tf	504.25	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.11	J/mol×K	877.76	Joback Method
cpg	1205.60	J/mol×K	1041.98	Joback Method
cpg	1191.91	J/mol×K	1009.14	Joback Method
cpg	1176.92	J/mol×K	976.29	Joback Method
cpg	1160.64	J/mol×K	943.45	Joback Method
cpg	1143.04	J/mol×K	910.60	Joback Method
cpg	1218.02	J/mol×K	1074.82	Joback Method
dvisc	0.0000295	Pa×s	877.76	Joback Method

dvisc	0.0000391	Pa×s	815.51	Joback Method
dvisc	0.0000543	Pa×s	753.26	Joback Method
dvisc	0.0000800	Pa×s	691.00	Joback Method
dvisc	0.0001273	Pa×s	628.75	Joback Method
dvisc	0.0002244	Pa×s	566.50	Joback Method
dvisc	0.0004546	Pa×s	504.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381959&Units=SI
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

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