Diglycolic acid, 2-pentyl tridecyl ester

Inchi: InChI=1S/C22H42O5/c1-4-6-7-8-9-10-11-12-13-14-15-17-26-21(23)18-25-19-22(24)27-2
InchiKey: KSYUVCVOLZJCPH-UHFFFAOYSA-N
Formula: C22H42O5
SMILES: CCCCCCCCCCCCCOC(=O)COCC(=O)OC(C)CCC
Mol. weight [g/mol]: 386.57

Physical Properties

Property code	Value	Unit	Source
gf	-440.92	kJ/mol	Joback Method
hf	-1124.51	kJ/mol	Joback Method
hfus	55.97	kJ/mol	Joback Method
hvap	84.90	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	5.589		Crippen Method
mcvol	341.590	ml/mol	McGowan Method
pc	948.50	kPa	Joback Method
rinpol	3153.00		NIST Webbook
rinpol	3153.00		NIST Webbook
tb	877.32	K	Joback Method
tc	1074.12	K	Joback Method
tf	489.25	K	Joback Method
vc	1.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.56	J/mol×K	877.32	Joback Method
cpg	1143.45	J/mol×K	910.12	Joback Method
cpg	1161.00	J/mol×K	942.92	Joback Method
cpg	1177.23	J/mol×K	975.72	Joback Method
cpg	1192.16	J/mol×K	1008.52	Joback Method
cpg	1205.79	J/mol×K	1041.32	Joback Method
cpg	1218.14	J/mol×K	1074.12	Joback Method
dvisc	0.0005231	Pa×s	489.25	Joback Method

dvisc	0.0002392	Pa×s	553.93	Joback Method
dvisc	0.0001288	Pa×s	618.61	Joback Method
dvisc	0.0000780	Pa×s	683.28	Joback Method
dvisc	0.0000515	Pa×s	747.96	Joback Method
dvisc	0.0000363	Pa×s	812.64	Joback Method
dvisc	0.0000270	Pa×s	877.32	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=U382344&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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