Diglycolic acid, neopentyl tetradecyl ester

Inchi: InChI=1S/C23H44O5/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-27-21(24)18-26-19-22(25)2
InchiKey: YUUVGIZDJOTVTR-UHFFFAOYSA-N
Formula: C23H44O5
SMILES: CCCCCCCCCCCCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 400.59

Physical Properties

Property code	Value	Unit	Source
gf	-427.22	kJ/mol	Joback Method
hf	-1148.62	kJ/mol	Joback Method
hfus	54.67	kJ/mol	Joback Method
hvap	86.22	kJ/mol	Joback Method
log10ws	-6.02		Crippen Method
logp	5.837		Crippen Method
mcvol	355.680	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	3246.00		NIST Webbook
rinpol	3246.00		NIST Webbook
tb	897.41	K	Joback Method
tc	1098.80	K	Joback Method
tf	517.94	K	Joback Method
vc	1.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1186.80	J/mol×K	897.41	Joback Method
cpg	1205.89	J/mol×K	930.98	Joback Method
cpg	1223.63	J/mol×K	964.54	Joback Method
cpg	1240.04	J/mol×K	998.11	Joback Method
cpg	1255.15	J/mol×K	1031.67	Joback Method
cpg	1269.01	J/mol×K	1065.24	Joback Method
cpg	1281.64	J/mol×K	1098.80	Joback Method
dvisc	0.0003645	Pa×s	517.94	Joback Method

dvisc	0.0001720	Pa×s	581.19	Joback Method
dvisc	0.0000940	Pa×s	644.43	Joback Method
dvisc	0.0000573	Pa×s	707.67	Joback Method
dvisc	0.0000378	Pa×s	770.92	Joback Method
dvisc	0.0000266	Pa×s	834.16	Joback Method
dvisc	0.0000197	Pa×s	897.41	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381926&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