Glycerol, 2,3-dimethyl, 1-(14-methylhexadecanoate)

Inchi: InChI=1S/C22H44O4/c1-5-20(2)16-14-12-10-8-6-7-9-11-13-15-17-22(23)26-19-21(25-4)1

InchiKey: BSEOPQDUVRJRND-UHFFFAOYSA-N

Formula: C22H44O4

SMILES: CCC(C)CCCCCCCCCCCCC(=O)OCC(COC)OC

Mol. weight [g/mol]: 372.58

Physical Properties

Property code	Value	Unit	Source
gf	-314.44	kJ/mol	Joback Method
hf	-1017.21	kJ/mol	Joback Method
hfus	50.85	kJ/mol	Joback Method
hvap	77.77	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.918		Crippen Method
mcvol	340.020	ml/mol	McGowan Method
pc	917.16	kPa	Joback Method
rinpol	2343.00		NIST Webbook
rinpol	2343.00		NIST Webbook
tb	823.01	K	Joback Method
tc	1008.16	K	Joback Method
tf	424.32	K	Joback Method
vc	1.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.11	J/mol×K	823.01	Joback Method
cpg	1119.50	J/mol×K	853.87	Joback Method
cpg	1138.69	J/mol×K	884.73	Joback Method
cpg	1156.68	J/mol×K	915.59	Joback Method
cpg	1173.50	J/mol×K	946.44	Joback Method
cpg	1189.15	J/mol×K	977.30	Joback Method
cpg	1203.65	J/mol×K	1008.16	Joback Method
dvisc	0.0008750	Pa×s	424.32	Joback Method

dvisc	0.0003285	Pa×s	490.77	Joback Method
dvisc	0.0001558	Pa×s	557.22	Joback Method
dvisc	0.0000866	Pa×s	623.66	Joback Method
dvisc	0.0000539	Pa×s	690.11	Joback Method
dvisc	0.0000365	Pa×s	756.56	Joback Method
dvisc	0.0000263	Pa×s	823.01	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=R56432&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