Glycerol, 2,3-dimethyl, 1-(13-methylpentadecanoate)

Inchi: InChI=1S/C21H42O4/c1-5-19(2)15-13-11-9-7-6-8-10-12-14-16-21(22)25-18-20(24-4)17-2

InchiKey: FETIKOHNKAOYHJ-UHFFFAOYSA-N

Formula: C21H42O4

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

Mol. weight [g/mol]: 358.56

Physical Properties

Property code	Value	Unit	Source
gf	-322.86	kJ/mol	Joback Method
hf	-996.57	kJ/mol	Joback Method
hfus	48.26	kJ/mol	Joback Method
hvap	75.54	kJ/mol	Joback Method
log10ws	-5.52		Crippen Method
logp	5.528		Crippen Method
mcvol	325.930	ml/mol	McGowan Method
pc	972.91	kPa	Joback Method
rinpol	2242.00		NIST Webbook
tb	800.13	K	Joback Method
tc	981.54	K	Joback Method
tf	413.05	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.84	J/mol×K	800.13	Joback Method
cpg	1056.80	J/mol×K	830.36	Joback Method
cpg	1075.65	J/mol×K	860.60	Joback Method
cpg	1093.38	J/mol×K	890.83	Joback Method
cpg	1110.01	J/mol×K	921.07	Joback Method
cpg	1125.56	J/mol×K	951.30	Joback Method
cpg	1140.02	J/mol×K	981.54	Joback Method
dvisc	0.0009966	Pa×s	413.05	Joback Method
dvisc	0.0003765	Pa×s	477.56	Joback Method

dvisc	0.0001794	Pa×s	542.08	Joback Method
dvisc	0.0001000	Pa×s	606.59	Joback Method
dvisc	0.0000624	Pa×s	671.10	Joback Method
dvisc	0.0000423	Pa×s	735.62	Joback Method
dvisc	0.0000305	Pa×s	800.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56414&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