Glycerol, 2,3-dimethyl, 1-hexadecanoate

Inchi: InChI=1S/C21H42O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21(22)25-19-20(24-3)18-2
InchiKey: UELIEEDDIWUFDH-UHFFFAOYSA-N
Formula: C21H42O4
SMILES: CCCCCCCCCCCCCCCC(=O)OCC(COC)OC
Mol. weight [g/mol]: 358.56

Physical Properties

Property code	Value	Unit	Source
gf	-320.42	kJ/mol	Joback Method
hf	-991.29	kJ/mol	Joback Method
hfus	51.79	kJ/mol	Joback Method
hvap	75.93	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	5.672		Crippen Method
mcvol	325.930	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
tb	800.57	K	Joback Method
tc	981.43	K	Joback Method
tf	428.05	K	Joback Method
vc	1.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1036.38	J/mol×K	800.57	Joback Method
cpg	1056.28	J/mol×K	830.71	Joback Method
cpg	1075.08	J/mol×K	860.86	Joback Method
cpg	1092.78	J/mol×K	891.00	Joback Method
cpg	1109.39	J/mol×K	921.14	Joback Method
cpg	1124.93	J/mol×K	951.29	Joback Method
cpg	1139.40	J/mol×K	981.43	Joback Method
dvisc	0.0008104	Pa×s	428.05	Joback Method

dvisc	0.0003397	Pa×s	490.14	Joback Method
dvisc	0.0001731	Pa×s	552.22	Joback Method
dvisc	0.0001011	Pa×s	614.31	Joback Method
dvisc	0.0000652	Pa×s	676.40	Joback Method
dvisc	0.0000452	Pa×s	738.48	Joback Method
dvisc	0.0000332	Pa×s	800.57	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56482&Units=SI

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