Glycerol, 2,3-dimethyl,1-tridecanoate

Inchi: InChI=1S/C18H36O4/c1-4-5-6-7-8-9-10-11-12-13-14-18(19)22-16-17(21-3)15-20-2/h17H
InchiKey: HTLXKLKWUKPYAP-UHFFFAOYSA-N
Formula: C18H36O4
SMILES: CCCCCCCCCCCCC(=O)OCC(COC)OC
Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	-345.68	kJ/mol	Joback Method
hf	-929.37	kJ/mol	Joback Method
hfus	44.02	kJ/mol	Joback Method
hvap	69.25	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	4.502		Crippen Method
mcvol	283.660	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	1972.00		NIST Webbook
tb	731.93	K	Joback Method
tc	905.00	K	Joback Method
tf	394.24	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.44	J/mol×K	731.93	Joback Method
cpg	873.04	J/mol×K	760.78	Joback Method
cpg	890.74	J/mol×K	789.62	Joback Method
cpg	907.55	J/mol×K	818.47	Joback Method
cpg	923.46	J/mol×K	847.31	Joback Method
cpg	938.49	J/mol×K	876.16	Joback Method
cpg	952.63	J/mol×K	905.00	Joback Method
dvisc	0.0011434	Pa×s	394.24	Joback Method
dvisc	0.0004929	Pa×s	450.52	Joback Method

dvisc	0.0002561	Pa×s	506.80	Joback Method
dvisc	0.0001517	Pa×s	563.09	Joback Method
dvisc	0.0000988	Pa×s	619.37	Joback Method
dvisc	0.0000691	Pa×s	675.65	Joback Method
dvisc	0.0000511	Pa×s	731.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56567&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