Glycerol, 2,3-dimethyl, 1-(11-methyldodecanoate)

Inchi: InChI=1S/C18H36O4/c1-16(2)12-10-8-6-5-7-9-11-13-18(19)22-15-17(21-4)14-20-3/h16-1

InchiKey: YFKZABLYWWSRQJ-UHFFFAOYSA-N

Formula: C18H36O4

SMILES: COCC(COC(=O)CCCCCCCCCC(C)C)OC

Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	-348.12	kJ/mol	Joback Method
hf	-934.65	kJ/mol	Joback Method
hfus	40.49	kJ/mol	Joback Method
hvap	68.86	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	4.358		Crippen Method
mcvol	283.660	ml/mol	McGowan Method
pc	1174.44	kPa	Joback Method
rinpol	1934.00		NIST Webbook
rinpol	1934.00		NIST Webbook
tb	731.49	K	Joback Method
tc	905.99	K	Joback Method
tf	379.24	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.89	J/mol×K	731.49	Joback Method
cpg	873.67	J/mol×K	760.57	Joback Method
cpg	891.52	J/mol×K	789.66	Joback Method
cpg	908.45	J/mol×K	818.74	Joback Method
cpg	924.47	J/mol×K	847.82	Joback Method
cpg	939.58	J/mol×K	876.90	Joback Method
cpg	953.78	J/mol×K	905.99	Joback Method
dvisc	0.0014422	Pa×s	379.24	Joback Method

dvisc	0.0005566	Pa×s	437.95	Joback Method
dvisc	0.0002690	Pa×s	496.66	Joback Method
dvisc	0.0001517	Pa×s	555.37	Joback Method
dvisc	0.0000954	Pa×s	614.07	Joback Method
dvisc	0.0000651	Pa×s	672.78	Joback Method
dvisc	0.0000472	Pa×s	731.49	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=R56389&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