Glycerol, 2,3-dimethyl, 1-(12-methyltridecanoate)

Inchi: InChI=1S/C19H38O4/c1-17(2)13-11-9-7-5-6-8-10-12-14-19(20)23-16-18(22-4)15-21-3/h1

InchiKey: ACLOHUMLCVGQGQ-UHFFFAOYSA-N

Formula: C19H38O4

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

Mol. weight [g/mol]: 330.50

Physical Properties

Property code	Value	Unit	Source
gf	-339.70	kJ/mol	Joback Method
hf	-955.29	kJ/mol	Joback Method
hfus	43.08	kJ/mol	Joback Method
hvap	71.09	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.748		Crippen Method
mcvol	297.750	ml/mol	McGowan Method
pc	1100.81	kPa	Joback Method
rinpol	2033.00		NIST Webbook
tb	754.37	K	Joback Method
tc	930.51	K	Joback Method
tf	390.51	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.65	J/mol×K	754.37	Joback Method
cpg	933.81	J/mol×K	783.73	Joback Method
cpg	951.99	J/mol×K	813.08	Joback Method
cpg	969.20	J/mol×K	842.44	Joback Method
cpg	985.44	J/mol×K	871.80	Joback Method
cpg	1000.72	J/mol×K	901.15	Joback Method
cpg	1015.03	J/mol×K	930.51	Joback Method
dvisc	0.0012798	Pa×s	390.51	Joback Method
dvisc	0.0004903	Pa×s	451.15	Joback Method

dvisc	0.0002358	Pa×s	511.80	Joback Method
dvisc	0.0001324	Pa×s	572.44	Joback Method
dvisc	0.0000830	Pa×s	633.08	Joback Method
dvisc	0.0000565	Pa×s	693.73	Joback Method
dvisc	0.0000409	Pa×s	754.37	Joback Method

Sources

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=R56400&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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