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

Inchi: InChI=1S/C20H40O4/c1-5-18(2)14-12-10-8-6-7-9-11-13-15-20(21)24-17-19(23-4)16-22-3

InchiKey: BGVGITAXRXEPPX-UHFFFAOYSA-N

Formula: C20H40O4

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

Mol. weight [g/mol]: 344.53

Physical Properties

Property code	Value	Unit	Source
gf	-331.28	kJ/mol	Joback Method
hf	-975.93	kJ/mol	Joback Method
hfus	45.67	kJ/mol	Joback Method
hvap	73.31	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	5.138		Crippen Method
mcvol	311.840	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rinpol	2143.00		NIST Webbook
tb	777.25	K	Joback Method
tc	955.67	K	Joback Method
tf	401.78	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	975.32	J/mol×K	777.25	Joback Method
cpg	994.88	J/mol×K	806.99	Joback Method
cpg	1013.39	J/mol×K	836.72	Joback Method
cpg	1030.87	J/mol×K	866.46	Joback Method
cpg	1047.31	J/mol×K	896.20	Joback Method
cpg	1062.73	J/mol×K	925.94	Joback Method
cpg	1077.13	J/mol×K	955.67	Joback Method
dvisc	0.0011313	Pa×s	401.78	Joback Method
dvisc	0.0004303	Pa×s	464.36	Joback Method

dvisc	0.0002059	Pa×s	526.94	Joback Method
dvisc	0.0001152	Pa×s	589.51	Joback Method
dvisc	0.0000721	Pa×s	652.09	Joback Method
dvisc	0.0000490	Pa×s	714.67	Joback Method
dvisc	0.0000354	Pa×s	777.25	Joback Method

Sources

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=R56393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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