

Glycerol, 2,3-dimethyl, 1-(13-methyltetradecanoate)

Inchi:	InChI=1S/C20H40O4/c1-18(2)14-12-10-8-6-5-7-9-11-13-15-20(21)24-17-19(23-4)16-22-3
InchiKey:	NJAUMMQNSFVTTN-UHFFFAOYSA-N
Formula:	C20H40O4
SMILES:	COCC(COC(=O)CCCCCCCCCCCC(C)C)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
mvol	311.840	ml/mol	McGowan Method
pc	1033.90	kPa	Joback Method
rmpol	2134.00		NIST Webbook
tb	777.25	K	Joback Method
tc	955.67	K	Joback Method
tf	401.78	K	Joback Method
vc	1.204	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002059	Paxs	526.94	Joback Method
dvisc	0.0001152	Paxs	589.51	Joback Method
dvisc	0.0000721	Paxs	652.09	Joback Method
dvisc	0.0000490	Paxs	714.67	Joback Method
dvisc	0.0000354	Paxs	777.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R56428&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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