Octadecanoic acid, 2,3-dihydroxypropyl ester

Other names:	Stearin, 1-mono- «alpha»-Monostearin Aldo MSD Aldo MSLG Aldo 33 Aldo 75 Arlacel 165 Emerest 2407 Glycerin 1-monostearate Glycerin 1-stearate Glycerol «alpha»-monostearate Glycerol 1-monostearate Glycerol 1-stearate Glyceryl 1-monostearate Sandin EU Stearic acid «alpha»-monoglyceride Stearic acid 1-monoglyceride Tegin 55G 1-Glyceryl stearate 1-Monostearin 1-Monostearoylglycerol 1,2,3-Propanetriol 1-octadecanoyl ester Glycerol «alpha»-sterate Monostearin (l) 3-Stearoyloxy-1,2-propanediol NSC 3875 Glyceryl 1-octadecanoate 2,3-Dihydroxypropyl stearate
Inchi:	InChI=1S/C21H42O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21(24)25-19-20(23)18
InchiKey:	VBICKXHEKHSIBG-UHFFFAOYSA-N
Formula:	C21H42O4
SMILES:	CCCCCCCCCCCCCCCCCC(=O)OCC(O)CO
Mol. weight [g/mol]:	358.56
CAS:	123-94-4

Physical Properties

Property code	Value	Unit	Source

chs	-12928.80 ± 1.80	kJ/mol	NIST Webbook
gf	-384.06	kJ/mol	Joback Method
hf	-1031.31	kJ/mol	Joback Method
hfs	-1337.80 ± 2.20	kJ/mol	NIST Webbook
hfus	57.59	kJ/mol	Joback Method
hvap	104.47	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.144		Crippen Method
mcvol	325.930	ml/mol	McGowan Method
pc	1114.08	kPa	Joback Method
tb	940.09	K	Joback Method
tc	1162.77	K	Joback Method
tf	347.20 ± 0.20	K	NIST Webbook
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.99	J/mol×K	940.09	Joback Method
cpg	1137.46	J/mol×K	977.20	Joback Method
cpg	1154.59	J/mol×K	1014.32	Joback Method
cpg	1170.45	J/mol×K	1051.43	Joback Method
cpg	1185.10	J/mol×K	1088.55	Joback Method
cpg	1198.59	J/mol×K	1125.66	Joback Method
cpg	1210.98	J/mol×K	1162.77	Joback Method
cps	610.40	J/mol×K	298.00	NIST Webbook
cps	866.00	J/mol×K	298.20	NIST Webbook
dvisc	0.0002903	Pa×s	505.23	Joback Method
dvisc	0.0000633	Pa×s	577.71	Joback Method
dvisc	0.0000194	Pa×s	650.18	Joback Method
dvisc	0.0000075	Pa×s	722.66	Joback Method
dvisc	0.0000035	Pa×s	795.14	Joback Method
dvisc	0.0000018	Pa×s	867.61	Joback Method
dvisc	0.0000011	Pa×s	940.09	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=C123944&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume