

Octadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester

Other names:

Stearin, 2-mono-
«beta»-Glyceryl monostearate
«beta»-Monostearin
Glycerol-«beta»-monostearate
Stearic acid «beta»-monoglyceride
2-Monostearin
2-Monostearoylglycerol
1,2,3-Propanetriol 2-octadecanoyl ester
Glycerol «beta»-sterate
2-Stearoylglycerol

Inchi: InChI=1S/C21H42O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-21(24)25-20(18-22)19

InchiKey: YQEMORVAKMFKLG-UHFFFAOYSA-N

Formula: C21H42O4

SMILES: CCCCCCCCCCCCCCCCCC(=O)OC(CO)CO

Mol. weight [g/mol]: 358.56

CAS: 621-61-4

Physical Properties

Property code	Value	Unit	Source
chs	-12944.80 ± 2.30	kJ/mol	NIST Webbook
gf	-384.06	kJ/mol	Joback Method
hf	-1031.31	kJ/mol	Joback Method
hfs	-1321.30 ± 2.60	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	505.23	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.99	J/molxK	940.09	Joback Method
cpg	1137.46	J/molxK	977.20	Joback Method
cpg	1154.59	J/molxK	1014.32	Joback Method
cpg	1170.45	J/molxK	1051.43	Joback Method
cpg	1185.10	J/molxK	1088.55	Joback Method
cpg	1198.59	J/molxK	1125.66	Joback Method
cpg	1210.98	J/molxK	1162.77	Joback Method
cps	610.40	J/molxK	298.00	NIST Webbook
dvisc	0.0002903	Paxs	505.23	Joback Method
dvisc	0.0000633	Paxs	577.71	Joback Method
dvisc	0.0000194	Paxs	650.18	Joback Method
dvisc	0.0000075	Paxs	722.66	Joback Method
dvisc	0.0000035	Paxs	795.14	Joback Method
dvisc	0.0000018	Paxs	867.61	Joback Method
dvisc	0.0000011	Paxs	940.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621614&Units=SI
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

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

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