

12-Hydroxystearic acid

Other names:	Octadecanoic acid, 12-hydroxy- Cerit Fac 3 Harwax A Hydrofol Acid 200 Stearic acid, 12-hydroxy- 12-Hydroxyoctadecanoic acid Barolub FTO Ceroxin GL KOW Loxiol G 21 DL-12-Hydroxystearic acid NSC 2385
Inchi:	InChI=1S/C18H36O3/c1-2-3-4-11-14-17(19)15-12-9-7-5-6-8-10-13-16-18(20)21/h17,19H
InchiKey:	ULQISTXYBZJSJ-UHFFFAOYSA-N
Formula:	C18H36O3
SMILES:	CCCCCCC(O)CCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	300.48
CAS:	106-14-9

Physical Properties

Property code	Value	Unit	Source
gf	-304.32	kJ/mol	Joback Method
hf	-837.17	kJ/mol	Joback Method
hfus	48.63	kJ/mol	Joback Method
hvap	95.38	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	5.303		Crippen Method
mcvol	277.790	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
tb	849.03	K	Joback Method
tc	1039.85	K	Joback Method
tf	449.19	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.88	J/molxK	849.03	Joback Method
cpg	922.00	J/molxK	880.83	Joback Method
cpg	937.24	J/molxK	912.64	Joback Method
cpg	951.63	J/molxK	944.44	Joback Method
cpg	965.21	J/molxK	976.24	Joback Method
cpg	978.04	J/molxK	1008.05	Joback Method
cpg	990.14	J/molxK	1039.85	Joback Method
dvisc	0.0012010	Paxs	449.19	Joback Method
dvisc	0.0002312	Paxs	515.83	Joback Method
dvisc	0.0000649	Paxs	582.47	Joback Method
dvisc	0.0000236	Paxs	649.11	Joback Method
dvisc	0.0000104	Paxs	715.75	Joback Method
dvisc	0.0000053	Paxs	782.39	Joback Method
dvisc	0.0000030	Paxs	849.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106149&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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