

12-HYDROXYSTERIC 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)CCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	300.48

Physical Properties

Property code	Value	Unit	Source
af	1.1898		Cheméo Relay (1.0)
gf	-304.32	kJ/mol	Joback Method
hf	-928.90	kJ/mol	Cheméo Relay (1.0)
hfus	48.63	kJ/mol	Joback Method
hvap	144.49	kJ/mol	Cheméo Relay (1.0)
ie	9.92	eV	Cheméo Relay (1.0)
log10ws	-4.55		Cheméo Relay (1.0)
logp	5.303		Crippen Method
mcvol	277.790	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
tb	623.26	K	Cheméo Relay (1.0)
tc	829.13	K	Cheméo Relay (1.0)
tf	369.49	K	Cheméo Relay (1.0)
vc	1.061	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106149&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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

h_{vap}:	Enthalpy of vaporization at standard conditions
i_e:	Ionization energy
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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