2,3-Dihydroxystearic acid

Inchi: InChI=1S/C18H36O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(19)17(20)18(21)22/h16-1
InchiKey: UAZFXPRZXKJSFJ-UHFFFAOYSA-N
Formula: C18H36O4
SMILES: CCCCCCCCCCCCCCCC(O)C(O)C(=O)O
Mol. weight [g/mol]: 316.48
CAS: 68601-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-443.58	kJ/mol	Joback Method
hf	-994.68	kJ/mol	Joback Method
hfus	49.19	kJ/mol	Joback Method
hvap	111.67	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.274		Crippen Method
mcvol	283.660	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
tb	940.77	K	Joback Method
tc	1163.12	K	Joback Method
tf	380.00 ± 2.00	K	NIST Webbook
tf	398.40 ± 1.00	K	NIST Webbook
tf	397.40 ± 2.00	K	NIST Webbook
tf	398.90 ± 2.00	K	NIST Webbook
tf	380.00 ± 1.50	K	NIST Webbook
vc	1.095	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.16	J/mol×K	940.77	Joback Method
cpg	985.06	J/mol×K	977.83	Joback Method
cpg	999.92	J/mol×K	1014.89	Joback Method
cpg	1013.79	J/mol×K	1051.95	Joback Method
cpg	1026.75	J/mol×K	1089.00	Joback Method

cpg	1038.87	J/mol×K	1126.06	Joback Method
cpg	1050.21	J/mol×K	1163.12	Joback Method
dvisc	0.0003443	Pa×s	495.01	Joback Method
dvisc	0.0000478	Pa×s	569.30	Joback Method
dvisc	0.0000105	Pa×s	643.60	Joback Method
dvisc	0.0000031	Pa×s	717.89	Joback Method
dvisc	0.0000012	Pa×s	792.18	Joback Method
dvisc	0.0000005	Pa×s	866.48	Joback Method
dvisc	0.0000003	Pa×s	940.77	Joback Method

Sources

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=C68601978&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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