Octadecanedioic acid

Other names:	Hexadecanedicarboxylic acid
	1,16-Hexadecanedicarboxylic acid
	1,18-Octadecadioic acid
	1,18-Octadecanedioic acid
Inchi:	InChI=1S/C18H34O4/c19-17(20)15-13-11-9-7-5-3-1-2-4-6-8-10-12-14-16-18(21)22/h1-16
InchiKey:	BNJOQKFENDDGSC-UHFFFAOYSA-N
Formula:	C18H34O4
SMILES:	O=C(O)CCCCCCCCCCCCCCCCC(=O)O
Mol. weight [g/mol]:	314.46
CAS:	871-70-5

Physical Properties

Property code	Value	Unit	Source
gf	-430.80	kJ/mol	Joback Method
hf	-944.47	kJ/mol	Joback Method
hfus	53.75	kJ/mol	Joback Method
hvap	102.51	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	5.397		Crippen Method
mcvol	279.360	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
tb	903.34	K	Joback Method
tc	1108.58	K	Joback Method
tf	398.10 ± 1.20	K	NIST Webbook
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.85	J/mol×K	903.34	Joback Method
cpg	938.03	J/mol×K	937.55	Joback Method
cpg	952.27	J/mol×K	971.75	Joback Method
cpg	965.61	J/mol×K	1005.96	Joback Method
cpg	978.10	J/mol×K	1040.17	Joback Method

cpg	989.80	J/mol×K	1074.37	Joback Method
cpg	1000.75	J/mol×K	1108.58	Joback Method
dvisc	0.0003702	Pa×s	514.12	Joback Method
dvisc	0.0001015	Pa×s	578.99	Joback Method
dvisc	0.0000361	Pa×s	643.86	Joback Method
dvisc	0.0000155	Pa×s	708.73	Joback Method
dvisc	0.0000077	Pa×s	773.60	Joback Method
dvisc	0.0000043	Pa×s	838.47	Joback Method
dvisc	0.0000026	Pa×s	903.34	Joback Method

Sources

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=C871705&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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