11-Octadecenoic acid, (Z)-

Other names: cis-Vaccenic acid
(Z)-11-Octadecenoic acid
cis-11-octadecenoic acid (asclepic acid)
Inchi: InChI=1S/C18H34O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h7-8H,2-6,9
InchiKey: UWHZIFQPPBDJPM-FPLPWBNLSA-N
Formula: C18H34O2
SMILES: CCCCCCC=CCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 282.46
CAS: 506-17-2

Physical Properties

Property code	Value	Unit	Source
gf	-84.84	kJ/mol	Joback Method
hf	-562.44	kJ/mol	Joback Method
hfus	48.26	kJ/mol	Joback Method
hvap	79.05	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	6.109		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
rinpol	2116.60		NIST Webbook
rinpol	2161.80		NIST Webbook
tb	761.45	K	Joback Method
tc	937.21	K	Joback Method
tf	284.40 ± 1.00	K	NIST Webbook
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.26	J/mol×K	937.21	Joback Method
cpg	811.35	J/mol×K	761.45	Joback Method
cpg	827.83	J/mol×K	790.74	Joback Method
cpg	843.52	J/mol×K	820.04	Joback Method

cpg	858.48	J/mol×K	849.33	Joback Method
cpg	872.72	J/mol×K	878.62	Joback Method
cpg	886.31	J/mol×K	907.92	Joback Method
dvisc	0.0000210	Pa×s	761.45	Joback Method
dvisc	0.0023727	Pa×s	398.29	Joback Method
dvisc	0.0006419	Pa×s	458.82	Joback Method
dvisc	0.0002355	Pa×s	519.34	Joback Method
dvisc	0.0001065	Pa×s	579.87	Joback Method
dvisc	0.0000560	Pa×s	640.40	Joback Method
dvisc	0.0000329	Pa×s	700.92	Joback Method
hfust	39.80	kJ/mol	287.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C506172&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
hfust: Enthalpy of fusion at a given temperature
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume