(9Z,11E)-Octadecadienoic acid

Inchi: InChI=1S/C18H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h7-10H,2-6,
InchiKey: JBYXPOFIGCOSSB-QRLRYFCNSA-N
Formula: C18H32O2
SMILES: CCCCCCC=CC=CCCCCCCCC(=O)O
Mol. weight [g/mol]: 280.45

Physical Properties

Property code	Value	Unit	Source
gf	-4.62	kJ/mol	Joback Method
hf	-445.22	kJ/mol	Joback Method
hfus	48.47	kJ/mol	Joback Method
hvap	79.00	kJ/mol	Joback Method
log10ws	-6.16		Crippen Method
logp	5.885		Crippen Method
mcvol	263.320	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	2110.00		NIST Webbook
rinpol	2110.00		NIST Webbook
tb	765.61	K	Joback Method
tc	944.34	K	Joback Method
tf	393.21	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	787.02	J/mol×K	765.61	Joback Method
cpg	802.93	J/mol×K	795.40	Joback Method
cpg	818.10	J/mol×K	825.19	Joback Method
cpg	832.56	J/mol×K	854.97	Joback Method
cpg	846.37	J/mol×K	884.76	Joback Method
cpg	859.57	J/mol×K	914.55	Joback Method
cpg	872.21	J/mol×K	944.34	Joback Method
dvisc	0.0023129	Pa×s	393.21	Joback Method

dvisc	0.0005934	Pa×s	455.28	Joback Method
dvisc	0.0002110	Pa×s	517.34	Joback Method
dvisc	0.0000937	Pa×s	579.41	Joback Method
dvisc	0.0000486	Pa×s	641.48	Joback Method
dvisc	0.0000284	Pa×s	703.54	Joback Method
dvisc	0.0000180	Pa×s	765.61	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R589549&Units=SI

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume