8-octadecenoic 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/h10-11H,2-9
InchiKey: WRIDQFICGBMAFQ-UHFFFAOYSA-N
Formula: C18H34O2
SMILES: CCCCCCCCCC=CCCCCCCC(=O)O
Mol. weight [g/mol]: 282.47
CAS: ---

Physical Properties

Property code	Value	Unit	Source
af	1.0298		Cheméo Relay (1.0)
gf	-84.84	kJ/mol	Joback Method
hf	-706.03	kJ/mol	Cheméo Relay (1.0)
hfus	48.26	kJ/mol	Joback Method
hvap	124.68	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-5.79		Cheméo Relay (1.0)
logp	6.109		Crippen Method
mcvol	267.620	ml/mol	McGowan Method
pc	1332.96	kPa	Joback Method
tb	606.18	K	Cheméo Relay (1.0)
tc	801.81	K	Cheméo Relay (1.0)
tf	318.52	K	Cheméo Relay (1.0)
vc	1.001	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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
cpg	899.26	J/mol×K	937.21	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
dvisc	0.0000210	Pa×s	761.45	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52924e+01
Coeff. B	-5.81882e+03
Coeff. C	-1.25923e+02
Temperature range (K), min.	514.15
Temperature range (K), max.	709.15

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume