8-hexadecenoic acid

Inchi: InChI=1S/C16H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h8-9H,2-7,10-15H
InchiKey: NJTVGRDDFBKQLU-UHFFFAOYSA-N
Formula: C16H30O2
SMILES: CCCCCCCC=CCCCCCCC(=O)O
Mol. weight [g/mol]: 254.41
CAS: ---

Physical Properties

Property code	Value	Unit	Source
af	0.9594		Cheméo Relay (1.0)
gf	-101.68	kJ/mol	Joback Method
hf	-663.41	kJ/mol	Cheméo Relay (1.0)
hfus	43.09	kJ/mol	Joback Method
hvap	116.18	kJ/mol	Cheméo Relay (1.0)
ie	9.15	eV	Cheméo Relay (1.0)
log10ws	-5.10		Cheméo Relay (1.0)
logp	5.328		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
tb	592.49	K	Cheméo Relay (1.0)
tc	784.20	K	Cheméo Relay (1.0)
tf	309.26	K	Cheméo Relay (1.0)
vc	0.889	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.79	J/mol×K	715.69	Joback Method
cpg	779.32	J/mol×K	887.89	Joback Method
cpg	767.14	J/mol×K	859.19	Joback Method
cpg	754.38	J/mol×K	830.49	Joback Method
cpg	740.99	J/mol×K	801.79	Joback Method
cpg	726.95	J/mol×K	773.09	Joback Method
cpg	712.23	J/mol×K	744.39	Joback Method

dvisc	0.0001549	Pa×s	545.72	Joback Method
dvisc	0.0000302	Pa×s	715.69	Joback Method
dvisc	0.0000474	Pa×s	659.03	Joback Method
dvisc	0.0000810	Pa×s	602.38	Joback Method
dvisc	0.0034930	Pa×s	375.75	Joback Method
dvisc	0.0003440	Pa×s	489.06	Joback Method
dvisc	0.0009417	Pa×s	432.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46024e+01
Coeff. B	-5.30092e+03
Coeff. C	-1.16610e+02
Temperature range (K), min.	486.92
Temperature range (K), max.	687.16

Sources

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

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

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

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

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