Hexadecenoic acid, Z-11-

Other names: Z-11-Hexadecenoic acid
Inchi: InChI=1S/C16H30O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h5-6H,2-4,7-15H2
InchiKey: JGMYDQCXGIMHLL-WAYWQWQTSA-N
Formula: C16H30O2
SMILES: CCCCC=CCCCCCCCCCC(=O)O
Mol. weight [g/mol]: 254.41
CAS: 2416-20-8

Physical Properties

Property code	Value	Unit	Source
gf	-101.68	kJ/mol	Joback Method
hf	-521.16	kJ/mol	Joback Method
hfus	43.09	kJ/mol	Joback Method
hvap	74.59	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	5.328		Crippen Method
mcvol	239.440	ml/mol	McGowan Method
pc	1541.49	kPa	Joback Method
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1953.00		NIST Webbook
tb	715.69	K	Joback Method
tc	887.89	K	Joback Method
tf	375.75	K	Joback Method
vc	0.936	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.79	J/mol×K	715.69	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
cpg	779.32	J/mol×K	887.89	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	0.0001549	Pa×s	545.72	Joback Method
dvisc	0.0003440	Pa×s	489.06	Joback Method
dvisc	0.0009417	Pa×s	432.41	Joback Method
dvisc	0.0034930	Pa×s	375.75	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=C2416208&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