3-hexadecenal, E

Other names: (E)-3-Hexadecenal
Inchi: InChI=1S/C16H30O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h13-14,16H,2-12,15H2
InchiKey: JQRGHGFKCUMTJM-BUHFOSPRSA-N
Formula: C16H30O
SMILES: CCCCCCCCCCCCC=CCC=O
Mol. weight [g/mol]: 238.41

Physical Properties

Property code	Value	Unit	Source
gf	64.54	kJ/mol	Joback Method
hf	-341.93	kJ/mol	Joback Method
hfus	39.69	kJ/mol	Joback Method
hvap	57.89	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	5.443		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	1808.00		NIST Webbook
ripol	2158.00		NIST Webbook
tb	618.30	K	Joback Method
tc	787.48	K	Joback Method
tf	307.00	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.39	J/mol×K	618.30	Joback Method
cpg	641.87	J/mol×K	646.50	Joback Method
cpg	658.57	J/mol×K	674.69	Joback Method
cpg	674.53	J/mol×K	702.89	Joback Method
cpg	689.77	J/mol×K	731.09	Joback Method
cpg	704.32	J/mol×K	759.29	Joback Method
cpg	718.22	J/mol×K	787.48	Joback Method

dvisc	0.0038359	Pa×s	307.00	Joback Method
dvisc	0.0015057	Pa×s	358.88	Joback Method
dvisc	0.0007485	Pa×s	410.77	Joback Method
dvisc	0.0004352	Pa×s	462.65	Joback Method
dvisc	0.0002823	Pa×s	514.53	Joback Method
dvisc	0.0001983	Pa×s	566.42	Joback Method
dvisc	0.0001477	Pa×s	618.30	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=R265273&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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