cis-11-Hexadecenal

Other names: 11-Hexadecenal, (Z)-
(Z)-11-Hexadecenal
Z-hexadec-11-enal
Inchi: InChI=1S/C16H30O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h5-6,16H,2-4,7-15H2,1
InchiKey: AMTITFMUKRZZEE-WAYWQWQTSA-N
Formula: C16H30O
SMILES: CCCCC=CCCCCCCCCCC=O
Mol. weight [g/mol]: 238.41
CAS: 53939-28-9

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	88.50	kJ/mol	NIST Webbook
log10ws	-5.65		Crippen Method
logp	5.443		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	1809.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1800.00		NIST Webbook
ripol	2159.00		NIST Webbook
ripol	2159.00		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	704.32	J/mol×K	759.29	Joback Method
cpg	689.77	J/mol×K	731.09	Joback Method
cpg	674.53	J/mol×K	702.89	Joback Method
cpg	658.57	J/mol×K	674.69	Joback Method
cpg	641.87	J/mol×K	646.50	Joback Method
cpg	718.22	J/mol×K	787.48	Joback Method
dvisc	0.0001477	Pa×s	618.30	Joback Method
dvisc	0.0001983	Pa×s	566.42	Joback Method
dvisc	0.0002823	Pa×s	514.53	Joback Method
dvisc	0.0004352	Pa×s	462.65	Joback Method
dvisc	0.0007485	Pa×s	410.77	Joback Method
dvisc	0.0015057	Pa×s	358.88	Joback Method
dvisc	0.0038359	Pa×s	307.00	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=C53939289&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