CIS-9-HEXADECENAL

Other names: 9-Hexadecenal, (Z)-
(Z)-9-Hexadecenal
(Z)-hexadec-9-enal
Inchi: InChI=1S/C16H30O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h7-8,16H,2-6,9-15H2,1
InchiKey: QFPVVMKZTVQDTL-FPLPWBNLSA-N
Formula: C16H30O
SMILES: CCCCCC/C=C\CCCCCCCC=O
Mol. weight [g/mol]: 238.42

Physical Properties

Property code	Value	Unit	Source
af	0.7163		Cheméo Relay (1.0)
gf	64.54	kJ/mol	Joback Method
hf	-397.34	kJ/mol	Cheméo Relay (1.0)
hfus	39.69	kJ/mol	Joback Method
hvap	88.00	kJ/mol	NIST Webbook
ie	8.97	eV	Cheméo Relay (1.0)
log10ws	-5.70		Cheméo Relay (1.0)
logp	5.443		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	1800.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1759.00		NIST Webbook
ripol	2147.00		NIST Webbook
tb	564.05	K	Cheméo Relay (1.0)
tc	756.93	K	Cheméo Relay (1.0)
tf	269.22	K	Cheméo Relay (1.0)
vc	0.873	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56219046&Units=SI

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

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
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