10-hexadecenal, Z

Other names: (Z)-10-Hexadecenal
Inchi: InChI=1S/C16H30O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h6-7,16H,2-5,8-15H2,1
InchiKey: NBLCOWKIHZCSCF-SREVYHEPSA-N
Formula: C16H30O
SMILES: CCCCCC=CCCCCCCCCC=O
Mol. weight [g/mol]: 238.41

Physical Properties

Property code	Value	Unit	Source
af	0.7165		Cheméo Relay (1.0)
gf	64.54	kJ/mol	Joback Method
hf	-415.27	kJ/mol	Cheméo Relay (1.0)
hfus	39.69	kJ/mol	Joback Method
hvap	87.40	kJ/mol	Cheméo Relay (1.0)
ie	8.95	eV	Cheméo Relay (1.0)
log10ws	-5.82		Cheméo Relay (1.0)
logp	5.443		Crippen Method
mcvol	233.570	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
ripol	2152.00		NIST Webbook
ripol	2152.00		NIST Webbook
tb	568.09	K	Cheméo Relay (1.0)
tc	758.92	K	Cheméo Relay (1.0)
tf	282.77	K	Cheméo Relay (1.0)
vc	0.882	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K

Coeff. A	-1.44380e+01
Coeff. B	1.51832e+00
Coeff. C	-9.23400e-04
Coeff. D	2.24500e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s
Coeff. A	-1.20320e+01
Coeff. B	1.98587e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	307.00
Temperature range (K), max.	551.42

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R265491&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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

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