Octadecanal

Other names:	Stearaldehyde
	Octadecyl aldehyde
	Stearyl aldehyde
	n-Octadecanal
	1-octadecanal
Inchi:	InChI=1S/C18H36O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h18H,2-17H2,1H
InchiKey:	FWWQKRXKHIRPJY-UHFFFAOYSA-N
Formula:	C18H36O
SMILES:	CCCCCCCCCCCCCCCCCC=O
Mol. weight [g/mol]:	268.48
CAS:	638-66-4

Physical Properties

Property code	Value	Unit	Source
gf	1.16	kJ/mol	Joback Method
hf	-500.43	kJ/mol	Joback Method
hfus	44.66	kJ/mol	Joback Method
hvap	62.38	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.447		Crippen Method
mcvol	266.050	ml/mol	McGowan Method
pc	1212.36	kPa	Joback Method
rinpol	2021.00		NIST Webbook
rinpol	2018.00		NIST Webbook
rinpol	2013.00		NIST Webbook
rinpol	2033.00		NIST Webbook
rinpol	2034.00		NIST Webbook
rinpol	2010.00		NIST Webbook
rinpol	2024.00		NIST Webbook
rinpol	1982.00		NIST Webbook
rinpol	2017.00		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	2012.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	1989.00		NIST Webbook
rinpol	1999.00		NIST Webbook

rinpol	2024.00		NIST Webbook
rinpol	2017.00		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	2016.00		NIST Webbook
rinpol	2017.00		NIST Webbook
rinpol	2037.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
rinpol	257.80		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	2043.00		NIST Webbook
rinpol	2038.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1995.00		NIST Webbook
rinpol	2002.00		NIST Webbook
rinpol	1976.00		NIST Webbook
rinpol	2018.00		NIST Webbook
ripol	2343.00		NIST Webbook
ripol	2390.00		NIST Webbook
ripol	2343.00		NIST Webbook
ripol	2388.00		NIST Webbook
ripol	2353.00		NIST Webbook
ripol	2357.00		NIST Webbook
ripol	2396.00		NIST Webbook
ripol	2396.00		NIST Webbook
ripol	2388.00		NIST Webbook
ripol	2336.00		NIST Webbook
ripol	2390.00		NIST Webbook
ripol	2380.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2400.00		NIST Webbook
tb	659.90	K	Joback Method
tc	824.47	K	Joback Method
tf	336.70 ± 20.00	K	NIST Webbook
tf	315.00 ± 3.00	K	NIST Webbook
tf	317.00 ± 5.00	K	NIST Webbook
tf	311.00 ± 4.00	K	NIST Webbook
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.78	J/mol×K	659.90	Joback Method
cpg	775.55	J/mol×K	687.33	Joback Method
cpg	793.51	J/mol×K	714.76	Joback Method
cpg	810.69	J/mol×K	742.18	Joback Method
cpg	827.12	J/mol×K	769.61	Joback Method
cpg	842.81	J/mol×K	797.04	Joback Method
cpg	857.81	J/mol×K	824.47	Joback Method
dvisc	0.0034940	Pa×s	334.62	Joback Method
dvisc	0.0013983	Pa×s	388.83	Joback Method
dvisc	0.0007002	Pa×s	443.05	Joback Method
dvisc	0.0004077	Pa×s	497.26	Joback Method
dvisc	0.0002640	Pa×s	551.47	Joback Method
dvisc	0.0001848	Pa×s	605.69	Joback Method
dvisc	0.0001371	Pa×s	659.90	Joback Method
hvapt	75.70	kJ/mol	514.50	NIST Webbook

Sources

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=C638664&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
hvapt: Enthalpy of vaporization at a given temperature

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