

17-Octadecenal

Inchi:	InChI=1S/C18H34O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h2,18H,1,3-17H
InchiKey:	MXCKZUNSOZSBPA-UHFFFAOYSA-N
Formula:	C18H34O
SMILES:	C=CCCCCCCCCCCCCCCC=O
Mol. weight [g/mol]:	266.46
CAS:	56554-86-0

Physical Properties

Property code	Value	Unit	Source
gf	89.00	kJ/mol	Joback Method
hf	-375.00	kJ/mol	Joback Method
hfus	43.38	kJ/mol	Joback Method
hvap	61.71	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.223		Crippen Method
mcvol	261.750	ml/mol	McGowan Method
pc	1248.61	kPa	Joback Method
tb	656.58	K	Joback Method
tc	822.72	K	Joback Method
tf	332.86	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.37	J/molxK	656.58	Joback Method
cpg	751.66	J/molxK	684.27	Joback Method
cpg	769.14	J/molxK	711.96	Joback Method
cpg	785.85	J/molxK	739.65	Joback Method
cpg	801.81	J/molxK	767.34	Joback Method
cpg	817.05	J/molxK	795.03	Joback Method
cpg	831.60	J/molxK	822.72	Joback Method
dvisc	0.0033854	Paxs	332.86	Joback Method
dvisc	0.0013851	Paxs	386.81	Joback Method

dvisc	0.0007053	Paxs	440.77	Joback Method
dvisc	0.0004161	Paxs	494.72	Joback Method
dvisc	0.0002723	Paxs	548.67	Joback Method
dvisc	0.0001923	Paxs	602.63	Joback Method
dvisc	0.0001438	Paxs	656.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C56554860&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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