

16-Octadecenal

Inchi:	InChI=1S/C18H34O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h2-3,18H,4-17H
InchiKey:	WTQUVMLIINDJCS-NSCUHMNNSA-N
Formula:	C18H34O
SMILES:	CC=CCCCCCCCCCCCCCC=O
Mol. weight [g/mol]:	266.46
CAS:	56554-87-1

Physical Properties

Property code	Value	Unit	Source
gf	81.38	kJ/mol	Joback Method
hf	-383.21	kJ/mol	Joback Method
hfus	44.87	kJ/mol	Joback Method
hvap	62.34	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	6.223		Crippen Method
mcvol	261.750	ml/mol	McGowan Method
pc	1257.48	kPa	Joback Method
tb	664.06	K	Joback Method
tc	833.01	K	Joback Method
tf	329.54	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.71	J/molxK	664.06	Joback Method
cpg	754.04	J/molxK	692.22	Joback Method
cpg	771.55	J/molxK	720.38	Joback Method
cpg	788.27	J/molxK	748.54	Joback Method
cpg	804.25	J/molxK	776.70	Joback Method
cpg	819.50	J/molxK	804.85	Joback Method
cpg	834.07	J/molxK	833.01	Joback Method
dvisc	0.0032761	Paxs	329.54	Joback Method
dvisc	0.0012611	Paxs	385.29	Joback Method

dvisc	0.0006179	Paxs	441.05	Joback Method
dvisc	0.0003554	Paxs	496.80	Joback Method
dvisc	0.0002285	Paxs	552.55	Joback Method
dvisc	0.0001593	Paxs	608.31	Joback Method
dvisc	0.0001180	Paxs	664.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56554871&Units=SI
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

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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