

(Z,Z)-9,12-Octadecadienal

Inchi:	InChI=1S/C18H32O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h6-7,9-10,18H,2
InchiKey:	HXLZULGRVFOIDK-HZJYTTRNSA-N
Formula:	C18H32O
SMILES:	CCCCC=CCC=CCCCCCCC=O
Mol. weight [g/mol]:	264.45

Physical Properties

Property code	Value	Unit	Source
gf	161.60	kJ/mol	Joback Method
hf	-265.99	kJ/mol	Joback Method
hfus	45.07	kJ/mol	Joback Method
hvap	62.30	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.999		Crippen Method
mcvol	257.450	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
rinpol	1971.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1971.00		NIST Webbook
tb	668.22	K	Joback Method
tc	841.93	K	Joback Method
tf	324.46	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.37	J/molxK	668.22	Joback Method
cpg	732.27	J/molxK	697.17	Joback Method
cpg	749.33	J/molxK	726.12	Joback Method
cpg	765.60	J/molxK	755.08	Joback Method
cpg	781.12	J/molxK	784.03	Joback Method
cpg	795.94	J/molxK	812.98	Joback Method
cpg	810.09	J/molxK	841.93	Joback Method

dvisc	0.0030745	Paxs	324.46	Joback Method
dvisc	0.0011371	Paxs	381.75	Joback Method
dvisc	0.0005452	Paxs	439.05	Joback Method
dvisc	0.0003097	Paxs	496.34	Joback Method
dvisc	0.0001978	Paxs	553.63	Joback Method
dvisc	0.0001374	Paxs	610.93	Joback Method
dvisc	0.0001016	Paxs	668.22	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=R584975&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
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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