9-Octadecenal

Other names: Octadecenyl aldehyde
Inchi: InChI=1S/C18H34O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h9-10,18H,2-8,1
InchiKey: ZENZJGDPWWLORF-MDZDMXLPSA-N
Formula: C18H34O
SMILES: CCCCCCCCC=CCCCCCCCC=O
Mol. weight [g/mol]: 266.46
CAS: 5090-41-5

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
rinpol	1993.00		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	2035.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2358.00		NIST Webbook
ripol	2375.00		NIST Webbook
ripol	2358.00		NIST Webbook
tb	664.06	K	Joback Method
tc	833.01	K	Joback Method
tf	329.54	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.71	J/mol×K	664.06	Joback Method

cpg	754.04	J/mol×K	692.22	Joback Method
cpg	771.55	J/mol×K	720.38	Joback Method
cpg	788.27	J/mol×K	748.54	Joback Method
cpg	804.25	J/mol×K	776.70	Joback Method
cpg	819.50	J/mol×K	804.85	Joback Method
cpg	834.07	J/mol×K	833.01	Joback Method
dvisc	0.0032761	Pa×s	329.54	Joback Method
dvisc	0.0012611	Pa×s	385.29	Joback Method
dvisc	0.0006179	Pa×s	441.05	Joback Method
dvisc	0.0003554	Pa×s	496.80	Joback Method
dvisc	0.0002285	Pa×s	552.55	Joback Method
dvisc	0.0001593	Pa×s	608.31	Joback Method
dvisc	0.0001180	Pa×s	664.06	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39541e+01
Coeff. B	-4.88551e+03
Coeff. C	-1.12440e+02
Temperature range (K), min.	469.92
Temperature range (K), max.	677.72

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5090415&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
pvap:	Vapor 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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