

9-Octadecynoic acid

Other names:	Stearolic acid octadec-9-ynoic acid
Inchi:	InChI=1S/C18H32O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h2-8,11-17H
InchiKey:	RGTIBVZDHOMOKC-UHFFFAOYSA-N
Formula:	C18H32O2
SMILES:	CCCCCCCCC#CCCCCCCCC(=O)O
Mol. weight [g/mol]:	280.45
CAS:	506-24-1

Physical Properties

Property code	Value	Unit	Source
gf	37.74	kJ/mol	Joback Method
hf	-407.36	kJ/mol	Joback Method
hfus	51.18	kJ/mol	Joback Method
hvap	81.24	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	5.556		Crippen Method
mvol	263.320	ml/mol	McGowan Method
pc	1444.64	kPa	Joback Method
rinpol	2184.00		NIST Webbook
tb	766.29	K	Joback Method
tc	947.07	K	Joback Method
tf	509.47	K	Joback Method
vc	1.030	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.27	J/molxK	766.29	Joback Method
cpg	804.47	J/molxK	796.42	Joback Method
cpg	819.87	J/molxK	826.55	Joback Method
cpg	834.50	J/molxK	856.68	Joback Method
cpg	848.39	J/molxK	886.81	Joback Method
cpg	861.58	J/molxK	916.94	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57549e+01
Coeff. B	-6.33546e+03
Coeff. C	-1.37536e+02
Temperature range (K), min.	547.14
Temperature range (K), max.	744.18

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback Method:

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

McGowan Method:

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

NIST Webbook:

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C506241&Units=SI>

Legend

cpg:	Ideal gas heat capacity
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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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