

9-Octadecanone

Inchi:	InChI=1S/C18H36O/c1-3-5-7-9-11-13-15-17-18(19)16-14-12-10-8-6-4-2/h3-17H2,1-2H3
InchiKey:	RPUZRNKKZZATGV-UHFFFAOYSA-N
Formula:	C18H36O
SMILES:	CCCCCCCCC(=O)CCCCCCCC
Mol. weight [g/mol]:	268.48
CAS:	18394-00-8

Physical Properties

Property code	Value	Unit	Source
gf	-28.24	kJ/mol	Joback Method
hf	-527.43	kJ/mol	Joback Method
hfus	43.97	kJ/mol	Joback Method
hvap	62.41	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	6.447		Crippen Method
mcvol	266.050	ml/mol	McGowan Method
pc	1203.12	kPa	Joback Method
tb	665.11	K	Joback Method
tc	832.25	K	Joback Method
tf	320.00 ± 3.00	K	NIST Webbook
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.85	J/mol×K	665.11	Joback Method
cpg	844.83	J/mol×K	804.39	Joback Method
cpg	828.99	J/mol×K	776.54	Joback Method
cpg	812.39	J/mol×K	748.68	Joback Method
cpg	795.03	J/mol×K	720.82	Joback Method
cpg	776.85	J/mol×K	692.97	Joback Method
cpg	859.94	J/mol×K	832.25	Joback Method
dvisc	0.0001238	Pa×s	665.11	Joback Method
dvisc	0.0001667	Pa×s	611.35	Joback Method

dvisc	0.0002378	Pa×s	557.59	Joback Method
dvisc	0.0003658	Pa×s	503.83	Joback Method
dvisc	0.0006238	Pa×s	450.07	Joback Method
dvisc	0.0012297	Pa×s	396.31	Joback Method
dvisc	0.0029992	Pa×s	342.55	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.48220e+01
Coeff. B	-5.11167e+03
Coeff. C	-1.08826e+02
Temperature range (K), min.	460.52
Temperature range (K), max.	646.30

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18394008&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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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