

3-Octadecanone

Other names:	octadecan-3-one
Inchi:	InChI=1S/C18H36O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)4-2/h3-17H2,1-2H3
InchiKey:	LMCGARAPKXJPNG-UHFFFAOYSA-N
Formula:	C18H36O
SMILES:	CCCCCCCCCCCCCCCC(=O)CC
Mol. weight [g/mol]:	268.48
CAS:	18261-92-2

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	342.55	K	Joback Method
vc	1.050	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.85	J/molxK	665.11	Joback Method
cpg	776.85	J/molxK	692.97	Joback Method
cpg	795.03	J/molxK	720.82	Joback Method
cpg	812.39	J/molxK	748.68	Joback Method
cpg	828.99	J/molxK	776.54	Joback Method
cpg	844.83	J/molxK	804.39	Joback Method
cpg	859.94	J/molxK	832.25	Joback Method
dvisc	0.0029992	Paxs	342.55	Joback Method

dvisc	0.0012297	Paxs	396.31	Joback Method
dvisc	0.0006238	Paxs	450.07	Joback Method
dvisc	0.0003658	Paxs	503.83	Joback Method
dvisc	0.0002378	Paxs	557.59	Joback Method
dvisc	0.0001667	Paxs	611.35	Joback Method
dvisc	0.0001238	Paxs	665.11	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	471.20	K	1.90	NIST Webbook

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

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=C18261922&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/73-823-7/3-Octadecanone.pdf>

Generated by Cheméo on 2024-04-25 22:10:56.267103855 +0000 UTC m=+16372305.187681168.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.