

9-Heptadecanone

Other names:	Di-n-octyl ketone Dioctyl ketone Octyl ketone Pelargone heptadecan-9-one
Inchi:	InChI=1S/C17H34O/c1-3-5-7-9-11-13-15-17(18)16-14-12-10-8-6-4-2/h3-16H2,1-2H3
InchiKey:	WTJKUFMLQLJOT-UHFFFAOYSA-N
Formula:	C17H34O
SMILES:	CCCCCCCCC(=O)CCCCCCCC
Mol. weight [g/mol]:	254.45
CAS:	540-08-9

Physical Properties

Property code	Value	Unit	Source
gf	-36.66	kJ/mol	Joback Method
hf	-506.79	kJ/mol	Joback Method
hfus	41.38	kJ/mol	Joback Method
hvap	60.18	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	6.057		Crippen Method
mcvol	251.960	ml/mol	McGowan Method
pc	1287.44	kPa	Joback Method
rinpol	1866.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1846.00		NIST Webbook
rinpol	1866.00		NIST Webbook
tb	524.70	K	NIST Webbook
tc	809.06	K	Joback Method
tf	324.00 ± 0.10	K	NIST Webbook
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.42	J/mol×K	753.45	Joback Method
cpg	800.76	J/mol×K	809.06	Joback Method
cpg	785.94	J/mol×K	781.26	Joback Method
cpg	700.79	J/mol×K	642.23	Joback Method
cpg	719.37	J/mol×K	670.04	Joback Method
cpg	737.15	J/mol×K	697.84	Joback Method
cpg	754.16	J/mol×K	725.65	Joback Method
dvisc	0.0001395	Paxs	642.23	Joback Method
dvisc	0.0002662	Paxs	538.58	Joback Method
dvisc	0.0001873	Paxs	590.40	Joback Method
dvisc	0.0032643	Paxs	331.28	Joback Method
dvisc	0.0013527	Paxs	383.11	Joback Method
dvisc	0.0006915	Paxs	434.93	Joback Method
dvisc	0.0004078	Paxs	486.75	Joback Method
hfust	66.68	kJ/mol	323.90	NIST Webbook
hfust	66.68	kJ/mol	323.90	NIST Webbook
hvapt	78.30	kJ/mol	460.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47284e+01
Coeff. B	-4.96373e+03
Coeff. C	-1.04850e+02
Temperature range (K), min.	448.58
Temperature range (K), max.	631.96

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=C540089&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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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