Methyl n-hexadecyl ketone

Other names: 2-Octadecanone
Inchi: InChI=1S/C18H36O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(2)19/h3-17H2,1-2H3
InchiKey: PJLJQAWUAPNCJC-UHFFFAOYSA-N
Formula: C18H36O
SMILES: CCCCCCCCCCCCCCCCC(C)=O
Mol. weight [g/mol]: 268.48
CAS: 7373-13-9

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
rinpol	1971.00		NIST Webbook
rinpol	1992.00		NIST Webbook
rinpol	333.26		NIST Webbook
rinpol	333.26		NIST Webbook
rinpol	1971.00		NIST Webbook
rinpol	2004.00		NIST Webbook
tb	665.11	K	Joback Method
tc	832.25	K	Joback Method
tf	300.40 ± 1.50	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(Pvp) = A + B/(T + C)
Coeff. A	1.49849e+01
Coeff. B	-5.18463e+03
Coeff. C	-1.09660e+02
Temperature range (K), min.	462.42
Temperature range (K), max.	645.63

Sources

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=C7373139&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume