2-Hexadecanone

Other names: Hexadecan-2-one
Inchi: InChI=1S/C16H32O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16(2)17/h3-15H2,1-2H3
InchiKey: XCXKZBWAKKPFCJ-UHFFFAOYSA-N
Formula: C16H32O
SMILES: CCCCCCCCCCCCCCC(C)=O
Mol. weight [g/mol]: 240.42
CAS: 18787-63-8

Physical Properties

Property code	Value	Unit	Source
gf	-45.08	kJ/mol	Joback Method
hf	-486.15	kJ/mol	Joback Method
hfus	38.80	kJ/mol	Joback Method
hvap	57.96	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.667		Crippen Method
mcvol	237.870	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	1782.00		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1791.00		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1782.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1808.00		NIST Webbook
rinpol	1807.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1783.00		NIST Webbook
rinpol	1804.00		NIST Webbook
rinpol	301.06		NIST Webbook

rinpol	1781.00		NIST Webbook
rinpol	1780.60		NIST Webbook
rinpol	1791.60		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1767.90		NIST Webbook
ripol	2150.00		NIST Webbook
ripol	2130.00		NIST Webbook
ripol	2112.00		NIST Webbook
ripol	2092.00		NIST Webbook
tb	619.35	K	Joback Method
tc	786.27	K	Joback Method
tf	320.01	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.73	J/mol×K	786.27	Joback Method
cpg	728.22	J/mol×K	758.45	Joback Method
cpg	713.03	J/mol×K	730.63	Joback Method
cpg	697.13	J/mol×K	702.81	Joback Method
cpg	680.51	J/mol×K	674.99	Joback Method
cpg	663.14	J/mol×K	647.17	Joback Method
cpg	645.00	J/mol×K	619.35	Joback Method
dvisc	0.0035270	Pa×s	320.01	Joback Method
dvisc	0.0001564	Pa×s	619.35	Joback Method
dvisc	0.0002094	Pa×s	569.46	Joback Method
dvisc	0.0002965	Pa×s	519.57	Joback Method
dvisc	0.0004520	Pa×s	469.68	Joback Method
dvisc	0.0007619	Pa×s	419.79	Joback Method
dvisc	0.0014783	Pa×s	369.90	Joback Method
hvapt	72.30	kJ/mol	481.00	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51347e+01
Coeff. B	-5.03598e+03
Coeff. C	-1.02432e+02
Temperature range (K), min.	441.62
Temperature range (K), max.	615.09

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18787638&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
hvapt:	Enthalpy of vaporization at a given temperature
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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