3-Hexadecanone

Other names: Ethyl n-tridecyl ketone
hexadecan-3-one
Inchi: InChI=1S/C16H32O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16(17)4-2/h3-15H2,1-2H3
InchiKey: LTMXHUUHBSCKEK-UHFFFAOYSA-N
Formula: C16H32O
SMILES: CCCCCCCCCCCCCC(=O)CC
Mol. weight [g/mol]: 240.42
CAS: 18787-64-9

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	1803.00		NIST Webbook
rinpol	1778.00		NIST Webbook
rinpol	1777.00		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	645.00	J/mol×K	619.35	Joback Method
cpg	663.14	J/mol×K	647.17	Joback Method
cpg	680.51	J/mol×K	674.99	Joback Method
cpg	697.13	J/mol×K	702.81	Joback Method

cpg	713.03	J/mol×K	730.63	Joback Method
cpg	728.22	J/mol×K	758.45	Joback Method
cpg	742.73	J/mol×K	786.27	Joback Method
dvisc	0.0035270	Pa×s	320.01	Joback Method
dvisc	0.0014783	Pa×s	369.90	Joback Method
dvisc	0.0007619	Pa×s	419.79	Joback Method
dvisc	0.0004520	Pa×s	469.68	Joback Method
dvisc	0.0002965	Pa×s	519.57	Joback Method
dvisc	0.0002094	Pa×s	569.46	Joback Method
dvisc	0.0001564	Pa×s	619.35	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	457.20	K	2.30	NIST Webbook
tbrp	413.20	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48723e+01
Coeff. B	-4.92228e+03
Coeff. C	-1.01264e+02
Temperature range (K), min.	438.76
Temperature range (K), max.	616.10

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18787649&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume