2-Pentadecanone

Other names:	2-pentandecanone
	Methyl tridecyl ketone
	Pentadecan-2-one
Inchi:	InChI=1S/C15H30O/c1-3-4-5-6-7-8-9-10-11-12-13-14-15(2)16/h3-14H2,1-2H3
InchiKey:	CJPNOLIZCWDHJK-UHFFFAOYSA-N
Formula:	C15H30O
SMILES:	CCCCCCCCCCCCCC(C)=O
Mol. weight [g/mol]:	226.40
CAS:	2345-28-0

Physical Properties

Property code	Value	Unit	Source
gf	-53.50	kJ/mol	Joback Method
hf	-465.51	kJ/mol	Joback Method
hfus	36.20	kJ/mol	Joback Method
hvap	55.73	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	5.277		Crippen Method
mcvol	223.780	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	286.58		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1679.00		NIST Webbook
rinpol	1690.90		NIST Webbook
rinpol	1688.00		NIST Webbook
ripol	2023.00		NIST Webbook
ripol	2011.00		NIST Webbook
tb	596.47	K	Joback Method
tc	763.83	K	Joback Method
tf	308.74	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.56	J/mol×K	596.47	Joback Method
cpg	671.69	J/mol×K	735.93	Joback Method
cpg	656.87	J/mol×K	708.04	Joback Method
cpg	641.36	J/mol×K	680.15	Joback Method
cpg	625.16	J/mol×K	652.26	Joback Method
cpg	608.23	J/mol×K	624.36	Joback Method
cpg	685.85	J/mol×K	763.83	Joback Method
dvisc	0.0001743	Pa×s	596.47	Joback Method
dvisc	0.0002327	Pa×s	548.52	Joback Method
dvisc	0.0003282	Pa×s	500.56	Joback Method
dvisc	0.0004978	Pa×s	452.61	Joback Method
dvisc	0.0008337	Pa×s	404.65	Joback Method
dvisc	0.0016037	Pa×s	356.69	Joback Method
dvisc	0.0037799	Pa×s	308.74	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51655e+01
Coeff. B	-4.94155e+03
Coeff. C	-9.86790e+01
Temperature range (K), min.	430.82
Temperature range (K), max.	600.16

Sources

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=C2345280&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

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