2-Naphthyl methyl ketone

Other names:	1-(2-Naphthalenyl)ethanone
	2'-Acetonaphthone
	2-Acetonaphthone
	2-Acetylnaphthalene
	Acetonaphthone
	Ethanone, 1-(2-naphthalenyl)-
	Ketone, methyl 2-naphthyl
	Methyl 2-naphthyl ketone
	Methyl «beta»-naphthyl ketone
	Methyl Â«betaÂ»-naphthyl ketone
	NSC 7658
	Oranger cyrstals
	«beta»-Acetonaphthalene
	«beta»-Acetonaphthone
	«beta»-Acetylnaphthalene
	«beta»-Methyl naphthyl ketone
	«beta»-Naphthyl methyl ketone
	Â«betaÂ»-Acetonaphthalene
	Â«betaÂ»-Acetonaphthone
	Â«betaÂ»-Acetylnaphthalene
	Â«betaÂ»-Methyl naphthyl ketone
	Â«betaÂ»-Naphthyl methyl ketone
Inchi:	InChI=1S/C12H10O/c1-9(13)11-7-6-10-4-2-3-5-12(10)8-11/h2-8H,1H3
InchiKey:	XSAYZAUNJMRRIR-UHFFFAOYSA-N
Formula:	C12H10O
SMILES:	CC(=O)c1ccc2ccccc2c1
Mol. weight [g/mol]:	170.21
CAS:	93-08-3

Physical Properties

Property code	Value	Unit	Source
gf	130.67	kJ/mol	Joback Method
hf	12.54	kJ/mol	Joback Method
hfus	19.11	kJ/mol	Joback Method
hvap	53.63	kJ/mol	Joback Method
ie	8.31	eV	NIST Webbook

log10ws	-3.94		Crippen Method
logp	3.042		Crippen Method
mcvol	138.290	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
rinpol	1598.40		NIST Webbook
rinpol	1604.00		NIST Webbook
tb	575.20	K	NIST Webbook
tb	573.70	K	NIST Webbook
tb	575.00 ± 1.00	K	NIST Webbook
tc	817.23	K	Joback Method
tf	325.20 ± 1.00	K	NIST Webbook
tf	329.00	K	NIST Webbook
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.12	J/mol×K	578.47	Joback Method
cpg	326.73	J/mol×K	618.26	Joback Method
cpg	339.29	J/mol×K	658.06	Joback Method
cpg	350.88	J/mol×K	697.85	Joback Method
cpg	361.57	J/mol×K	737.64	Joback Method
cpg	371.43	J/mol×K	777.44	Joback Method
cpg	380.56	J/mol×K	817.23	Joback Method
dvisc	0.0011679	Pa×s	385.22	Joback Method
dvisc	0.0017370	Pa×s	346.57	Joback Method
dvisc	0.0008442	Pa×s	423.87	Joback Method
dvisc	0.0006442	Pa×s	462.52	Joback Method
dvisc	0.0005126	Pa×s	501.17	Joback Method
dvisc	0.0004214	Pa×s	539.82	Joback Method
dvisc	0.0003556	Pa×s	578.47	Joback Method
hsubt	87.86 ± 0.42	kJ/mol	328.80	NIST Webbook
hsubt	87.90 ± 0.40	kJ/mol	305.50	NIST Webbook
hvapt	74.10	kJ/mol	483.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	445.20	K	2.30	NIST Webbook
tbrp	445.00 ± 1.00	K	2.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.09370e+01
Coeff. B	-9.89570e+03
Coeff. C	3.27040e+01
Temperature range (K), min.	446.52
Temperature range (K), max.	600.60

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C93083&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

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

hsubt: Enthalpy of sublimation at a given temperature

hvap: Enthalpy of vaporization at standard conditions

hvapt: Enthalpy of vaporization at a given temperature

ie: Ionization energy

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

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