Ethanone, 1-(1-Naphthalenyl)-

Other names:	1'-Acetonaphthone
	1-(1-Naphthalenyl)ethanone
	1-(Naphthalen-4-yl)ethanone
	1-Acetonaphthalene
	1-Acetonaphthone
	1-Acetylnaphthalene
	1-Naphthyl methyl ketone
	Methyl 1-naphthyl ketone
	Methyl «alpha»-naphthyl ketone
	Methyl Â«alphaÂ»-naphthyl ketone
	NSC 7659
	«alpha»-Acetonaphthone
	«alpha»-Acetylnaphthalene
	«alpha»-Methyl naphthyl ketone
	«alpha»-Naphthyl methyl ketone
	Â«alphaÂ»-Acetonaphthone
	Â«alphaÂ»-Acetylnaphthalene
	Â«alphaÂ»-Methyl naphthyl ketone
	Â«alphaÂ»-Naphthyl methyl ketone
Inchi:	InChI=1S/C12H10O/c1-9(13)11-8-4-6-10-5-2-3-7-12(10)11/h2-8H,1H3
InchiKey:	QQLIGMASAVJVON-UHFFFAOYSA-N
Formula:	C12H10O
SMILES:	CC(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	170.21
CAS:	941-98-0

Physical Properties

Property code	Value	Unit	Source
ea	0.60 ± 0.03	eV	NIST Webbook
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	8.23	eV	NIST Webbook
ie	8.23	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	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook
ripol	2471.00		NIST Webbook
ripol	2471.00		NIST Webbook
tb	575.20	K	NIST Webbook
tc	817.23	K	Joback Method
tf	307.00	K	NIST Webbook
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.56	J/mol×K	817.23	Joback Method
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
dvisc	0.0003556	Pa×s	578.47	Joback Method
dvisc	0.0017370	Pa×s	346.57	Joback Method
dvisc	0.0011679	Pa×s	385.22	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
hvapt	65.40	kJ/mol	478.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.50 ± 1.50	K	2.00	NIST Webbook
tbrp	417.00 ± 1.00	K	0.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.85376e+01
Coeff. B	-7.98937e+03
Coeff. C	3.83100e+00
Temperature range (K), min.	433.94
Temperature range (K), max.	600.23

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=C941980&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
ea:	Electron affinity
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
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
ripol:	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