1-Adamantyl methyl ketone

Other names:	Ethanone, 1-tricyclo[3.3.1.1(3,7)-]dec-1-yl-
	Ethanone, 1-tricyclo[3.3.1.13,7]dec-1-yl-
	Ketone, 1-adamantyl methyl
	1-(1-Adamantyl)ethanone
	1-Acetyladamantane
	Adamantyl methyl ketone
	Methyl 1-adamantyl ketone
	1-Adamantan-1-yl-ethanone
	Methyl adamantyl-1 ketone
	1-methyl adamantyl ketone
	Adamantane, 1-acetyl
	methyl tricyclo[3.3.1.13,7]dec-1-yl ketone
Inchi:	InChI=1S/C12H18O/c1-8(13)12-5-9-2-10(6-12)4-11(3-9)7-12/h9-11H,2-7H2,1H3
InchiKey:	DACIGVIOAFXPHW-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CC(=O)C12CC3CC(CC(C3)C1)C2
Mol. weight [g/mol]:	178.27
CAS:	1660-04-4

Physical Properties

Property code	Value	Unit	Source
affp	864.90	kJ/mol	NIST Webbook
basg	833.10	kJ/mol	NIST Webbook
chs	-6912.10 ± 2.60	kJ/mol	NIST Webbook
gf	78.19	kJ/mol	Joback Method
hf	-298.30 ± 3.20	kJ/mol	NIST Webbook
hfs	-382.50 ± 3.10	kJ/mol	NIST Webbook
hfus	15.51	kJ/mol	Joback Method
hsub	84.20 ± 0.60	kJ/mol	NIST Webbook
hsub	84.20 ± 0.60	kJ/mol	NIST Webbook
hvap	47.50	kJ/mol	Joback Method
ie	8.82 ± 0.05	eV	NIST Webbook
log10ws	-2.84		Crippen Method
logp	2.792		Crippen Method
mcvol	148.930	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
rinpol	1476.00		NIST Webbook

rinpol	1491.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1430.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1430.00		NIST Webbook
tb	547.89	K	Joback Method
tc	773.67	K	Joback Method
tf	344.89	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.63	J/mol×K	736.04	Joback Method
cpg	396.75	J/mol×K	547.89	Joback Method
cpg	416.77	J/mol×K	585.52	Joback Method
cpg	435.26	J/mol×K	623.15	Joback Method
cpg	452.43	J/mol×K	660.78	Joback Method
cpg	468.48	J/mol×K	698.41	Joback Method
cpg	498.09	J/mol×K	773.67	Joback Method
cps	217.50	J/mol×K	298.15	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1660044&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume