

Carbazol-1(2H)-one, 3,4-dihydro-6-methyl-

Other names:	1-keto-1,2,3,4-tetrahydro-6-methylcarbazole 6-methyl-2,3,4,9-tetrahydro-1H-carbazol-1-one
Inchi:	InChI=1S/C13H13NO/c1-8-5-6-11-10(7-8)9-3-2-4-12(15)13(9)14-11/h5-7,14H,2-4H2,1H3
InchiKey:	ITWUGZSJDMBOPH-UHFFFAOYSA-N
Formula:	C13H13NO
SMILES:	Cc1ccc2[nH]c3c(c2c1)CCCC3=O
Mol. weight [g/mol]:	199.25
CAS:	3449-48-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.33		Crippen Method
logp	2.513		Crippen Method
mcvol	155.800	ml/mol	McGowan Method
tf	468.45	K	Solubility and Metastable Zone Width of 1-Keto-1,2,3,4-tetrahydro-6-methylcarbazole in Acetone

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	26.90	kJ/mol	468.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3449487&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility and Metastable Zone Width of 1-Keto-1,2,3,4-tetrahydro-6-methylcarbazole in Acetone:	https://www.doi.org/10.1021/je0600552

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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