Carbazole, tetrahydro-9-acetyl-

Other names:	9-Acetyl-2,3,4,9-tetrahydro-1H-carbazole
	9H-Carbazole, 9-acetyl-1,2,3,4-tetrahydro-
	N-Acetyl-tetrahydrocarbazole
Inchi:	InChI=1S/C14H15NO/c1-10(16)15-13-8-4-2-6-11(13)12-7-3-5-9-14(12)15/h2,4,6,8H,3,5,7
InchiKey:	NAKAGIJKYRVETG-UHFFFAOYSA-N
Formula:	C14H15NO
SMILES:	CC(=O)n1c2c(c3ccccc31)CCCC2
Mol. weight [g/mol]:	213.28
CAS:	27236-49-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.89		Crippen Method
logp	3.180		Crippen Method
mcvol	169.890	ml/mol	McGowan Method
rinpol	2031.00		NIST Webbook
rinpol	2031.00		NIST Webbook
ripol	3078.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27236493&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices

ripol: Polar retention indices