

6,11-Dihydro-6,11-dioxo-5a,12-diazabenzob[b]cycloheptano [a]-indene

Inchi:	InChI=1S/C16H14N2O2/c19-15-10-6-3-4-7-11(10)16(20)14-13(15)17-12-8-2-1-5-9-18(12)
InchiKey:	UWKDSXGQTWYWMY-UHFFFAOYSA-N
Formula:	C16H14N2O2
SMILES:	O=C1c2ccccc2C(=O)c2c1nc1n2CCCCC1
Mol. weight [g/mol]:	266.29
CAS:	97999-91-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.78		Crippen Method
logp	2.385		Crippen Method
mcvol	194.460	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C97999912&Units=SI

Legend

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

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