6,11-Dihydro-6,11-dioxo-5a,12-diazabenzo[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/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=C97999912&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume