3H-1,4-benzodiazepine-2,5-dione, 8-chloro-1,2,4,5-tetrahydro-1,4-dimethyl-

Inchi: InChI=1S/C11H11ClN2O2/c1-13-6-10(15)14(2)9-5-7(12)3-4-8(9)11(13)16/h3-5H,6H2,1-2

InchiKey: PGBANJSYEASTRN-UHFFFAOYSA-N

Formula: C11H11ClN2O2

SMILES: CN1CC(=O)N(C)c2cc(Cl)ccc2C1=O

Mol. weight [g/mol]: 238.67

CAS: 1018-73-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	1.388		Crippen Method
mcvol	166.570	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=C1018731&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume