3H-1,4-benzodiazepine-2,5-dione,4-(p-chlorophen

Inchi: InChI=1S/C16H13ClN2O2/c1-18-14-5-3-2-4-13(14)16(21)19(10-15(18)20)12-8-6-11(17)7
InchiKey: JNLDODBGVIFIPV-UHFFFAOYSA-N
Formula: C16H13ClN2O2
SMILES: CN1C(=O)CN(c2ccc(Cl)cc2)C(=O)c2ccccc21
Mol. weight [g/mol]: 300.74
CAS: 1036-16-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	2.963		Crippen Method
mcvol	213.260	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1036164&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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