

NORCHLORDIAZEPOXIDE

Inchi: InChI=1S/C15H11ClN2O/c16-12-6-7-14-13(10-12)15(18(19)9-8-17-14)11-4-2-1-3-5-11/h
InchiKey: YIXUNVZJCJYWIW-UHFFFAOYSA-N
Formula: C15H11ClN2O
SMILES: [O-][N+]1=C(c2ccccc2)c2cc(Cl)ccc2N=CC1
Mol. weight [g/mol]: 270.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Cheméo Relay (1.0)
logp	3.404		Crippen Method
mcvol	193.300	ml/mol	McGowan Method
tf	438.14	K	Cheméo Relay (1.0)

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C16300257&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point

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