Panidazole

Inchi: InChI=1S/C11H12N4O2/c1-9-13-8-11(15(16)17)14(9)7-4-10-2-5-12-6-3-10/h2-3,5-6,8H,4
InchiKey: ARYPMCPJIWUCIP-UHFFFAOYSA-N
Formula: C11H12N4O2
SMILES: Cc1ncc([N+](=O)[O-])n1CCc1ccncc1
Mol. weight [g/mol]: 232.24
CAS: 13752-33-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.01		Crippen Method
logp	1.737		Crippen Method
mcvol	169.990	ml/mol	McGowan Method
rinpol	2065.00		NIST Webbook
rinpol	2065.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13752335&Units=SI
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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices