Simetryn

Inchi: InChI=1S/C8H15N5S/c1-12(2)6-9-7(13(3)4)11-8(10-6)14-5/h1-5H3
InchiKey: PRLMFHYBTOQSLN-UHFFFAOYSA-N
Formula: C8H15N5S
SMILES: CSc1nc(N(C)C)nc(N(C)C)n1
Mol. weight [g/mol]: 213.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Aqueous Solubility Prediction Method
log10ws	-2.68		Estimated Solubility Method
logp	0.725		Crippen Method
mcvol	166.070	ml/mol	McGowan Method
tf	355.65	K	Aqueous Solubility Prediction Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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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