Apazone

Inchi: InChI=1S/C16H20N4O2/c1-5-6-11-14(21)19-13-9-10(2)7-8-12(13)17-16(18(3)4)20(19)15
InchiKey: MPHPHYZQRGLTBO-UHFFFAOYSA-N
Formula: C16H20N4O2
SMILES: CCCC1C(=O)N2C(N(C)C)=Nc3ccc(C)cc3N2C1=O
Mol. weight [g/mol]: 300.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Aqueous Solubility Prediction Method
log10ws	-3.54		Estimated Solubility Method
logp	2.064		Crippen Method
mcvol	229.580	ml/mol	McGowan Method
tf	507.48	K	Aqueous Solubility Prediction Method

Sources

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
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
tf: Normal melting (fusion) point

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