

alprenolol

Inchi: InChI=1S/C18H28N2O/c1-4-5-12-20-13-7-6-11-16(20)18(21)19-17-14(2)9-8-10-15(17)3/
InchiKey: LEBVLXFERQHONN-UHFFFAOYSA-N
Formula: C18H28N2O
SMILES: CCCCN1CCCCC1C(=O)Nc1c(C)cccc1C
Mol. weight [g/mol]: 288.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Aqueous Solubility Prediction Method
logp	3.897		Crippen Method
mcvol	251.390	ml/mol	McGowan Method
tf	380.40	K	Aqueous Solubility Prediction Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>
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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