

Benzylpiperazine-M (OH-) isomer-2, 2AC

Inchi: InChI=1S/C15H20N2O3/c1-12(18)17-9-7-16(8-10-17)11-14-5-3-4-6-15(14)20-13(2)19/h3
InchiKey: JDIBNHDMHADMF3-UHFFFAOYSA-N
Formula: C15H20N2O3
SMILES: CC(=O)Oc1ccccc1CN1CCN(C(C)=O)CC1
Mol. weight [g/mol]: 276.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.99		Crippen Method
logp	1.276		Crippen Method
mcvol	216.560	ml/mol	McGowan Method
rinpol	2275.00		NIST Webbook
rinpol	2275.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R284318&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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