

Benzylpiperazine-M (OH-) isomer-1, 2AC

Inchi:	InChI=1S/C15H20N2O3/c1-12(18)17-9-7-16(8-10-17)11-14-3-5-15(6-4-14)20-13(2)19/h3
InchiKey:	MZAUTFBATWHAKF-UHFFFAOYSA-N
Formula:	C15H20N2O3
SMILES:	CC(=O)Oc1ccc(CN2CCN(C(C)=O)CC2)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
rinsol	2245.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R284303&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
rinsol:	Non-polar retention indices

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