Benzylpiperazine-M (HO-methoxy-), 2AC

Inchi: InChI=1S/C16H22N2O4/c1-12(19)18-8-6-17(7-9-18)11-14-4-5-15(22-13(2)20)10-16(14)2
InchiKey: OPTSUHFXPMJEII-UHFFFAOYSA-N
Formula: C16H22N2O4
SMILES: COc1cc(OC(C)=O)ccc1CN1CCN(C(C)=O)CC1
Mol. weight [g/mol]: 306.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.11		Crippen Method
logp	1.285		Crippen Method
mcvol	236.520	ml/mol	McGowan Method
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R284294&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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