

Bitertanol, isomer 1

Inchi: InChI=1S/C20H23N3O2/c1-20(2,3)18(24)19(23-14-21-13-22-23)25-17-11-9-16(10-12-17)
InchiKey: VGPIBGGRCVEHQZ-MOPGFXCFS-A-N
Formula: C₂₀H₂₃N₃O₂
SMILES: CC(C)(C)C(O)C(Oc1ccc(-c2ccccc2)cc1)n1cncn1
Mol. weight [g/mol]: 337.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.48		Crippen Method
logp	3.930		Crippen Method
mcvol	267.360	ml/mol	McGowan Method
rinpol	2695.00		NIST Webbook
rinpol	2700.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R566011&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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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<https://www.chemeo.com/cid/30-976-5/Bitertanol-isomer-1.pdf>

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