

Ormosanine I

Inchi: InChI=1S/C20H35N3/c1-3-9-21-18(8-1)20-13-16(12-15-6-5-10-22-19(15)20)17-7-2-4-11-
InchiKey: YUKCLPPRYNXRAF-UHFFFAOYSA-N
Formula: C20H35N3
SMILES: C1CCC(C23CC(CC4CCCNC42)C2CCCCN2C3)NC1
Mol. weight [g/mol]: 317.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	2.761		Crippen Method
mcvol	268.300	ml/mol	McGowan Method
rinpola	2487.00		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=R504860&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/62-281-1/Ormosanine-I.pdf>

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