

Ethylisobutrazine

Inchi: InChI=1S/C20H26N2S/c1-5-16-10-11-20-18(12-16)22(14-15(2)13-21(3)4)17-8-6-7-9-19(20)
InchiKey: USKHCLAXJXCWMO-UHFFFAOYSA-N
Formula: C20H26N2S
SMILES: CCc1ccc2c(c1)N(CC(C)CN(C)C)c1ccccc1S2
Mol. weight [g/mol]: 326.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	5.049		Crippen Method
mcvol	270.590	ml/mol	McGowan Method
rinpol	2455.00		NIST Webbook
rinpol	2455.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R67&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/68-702-7/Ethylisobutrazine.pdf>

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