

dehydropanamine-type

Inchi: InChI=1S/C20H31N3/c1-2-9-22-13-20-12-15(16(22)6-1)11-14-5-4-10-23(19(14)20)18-8-3
InchiKey: KNWAHXHMMOLUAW-NSDIEPNESA-N
Formula: C20H31N3
SMILES: C1=C2CCCN3C4CCCC(N4)C4(CC1C1CCCN1C4)C23
Mol. weight [g/mol]: 313.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Crippen Method
logp	2.733		Crippen Method
mcvol	253.140	ml/mol	McGowan Method
rinpol	2545.00		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=R322133&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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<https://www.chemeo.com/cid/53-886-0/dehydropanamine-type.pdf>

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