

Pyrrolidine, 1-tricyclo[4.3.1.12,5]undec-10-yl-, stereoisomer

Other names: 1-Tricyclo[4.3.1.1(2,5)]undec-10-ylpyrrolidine
Inchi: InChI=1S/C15H25N/c1-2-9-16(8-1)15-13-4-3-5-14(15)12-7-6-11(13)10-12/h11-15H,1-10H
InchiKey: FUCAIEMNUXSMGQ-UHFFFAOYSA-N
Formula: C15H25N
SMILES: C1CC2C3CCC(C3)C(C1)C2N1CCCC1
Mol. weight [g/mol]: 219.37
CAS: 85538-51-8

Physical Properties

Property code	Value	Unit	Source
ie	7.30	eV	NIST Webbook
ie	7.93	eV	NIST Webbook
log10ws	-3.40		Crippen Method
logp	3.297		Crippen Method
mcvol	188.750	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=C85538518&Units=SI>

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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