

Dodecahydro-1H,6H,11H-triopyrido[1,2-a:1',2'-c:1'',

Other names: Tripiperidine[trimer of 2,3,4,5-tetrahydropyridine]
Inchi: InChI=1S/C15H27N3/c1-4-10-16-13(7-1)17-11-5-2-9-15(17)18-12-6-3-8-14(16)18/h13-15
InchiKey: DKOLZPGCABHTDG-UHFFFAOYSA-N
Formula: C15H27N3
SMILES: C1CCN2C(C1)N1CCCCC1N1CCCCC21
Mol. weight [g/mol]: 249.40
CAS: 522-33-8

Physical Properties

Property code	Value	Unit	Source
ie	7.60	eV	NIST Webbook
ie	7.85	eV	NIST Webbook
log10ws	-3.21		Crippen Method
logp	2.436		Crippen Method
mcvol	208.710	ml/mol	McGowan Method

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=C522338&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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