

7,14-Methano-2H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazododecahydro-«beta»-Isosparteine

Other names: «beta»-Isosparteine
InChI: InChI=1S/C15H26N2/c1-3-7-16-11-13-9-12(14(16)5-1)10-17-8-4-2-6-15(13)17/h12-15H,1

[7S-(7«alpha»,7a«beta»,14«alpha»,14a«beta»)]-

Formula: C15H26N2
SMILES: C1CCN2CC3CC(CN4CCCCC34)C2C1
Mol. weight [g/mol]: 234.38
CAS: 24915-04-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	2.345		Crippen Method
mcvol	198.730	ml/mol	McGowan Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C24915046&Units=SI>
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>

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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