

Sparteine

Other names:

(-)-Sparteine

6«beta»,7«alpha»,9«alpha»,11«alpha»-Pachycarpine

6Â«betaÂ»,7Â«alphaÂ»,9Â«alphaÂ»,11Â«alphaÂ»-Pachycarpine

7,14-Methano-2H,6H-dipyrido(1,2-a:1',2'-e)(1,5)diazocine, dodecahydro-

7,14-Methano-2H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazocine, dodecahydro-

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

7,14-Methano-2H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazocine, dodecahydro-

[7S-(7Â«alphaÂ»,7aÂ«alphaÂ»,14Â«alphaÂ»,14aÂ«betaÂ»)]-

Dodecahydro

[7S-(7«alpha»,7a«alpha»,14«alpha»,14a«beta»)]-7,14-methano-2H,6H-dipyrido[1,2-a:1'

Dodecahydro

[7S-(7Â«alphaÂ»,7aÂ«alphaÂ»,14Â«alphaÂ»,14aÂ«betaÂ»)]-7,14-methano-2H,6H-dipy

L-sparteine

Lupinidin

Lupinidine

Sparteine

Sparteinum

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

InchiKey: SLRCCWJSBJZJBV-PYHGIMPFSAN

Formula: C15H26N2

SMILES: C1CCN2CC3CC(CN4CCCC34)C2C1

Mol. weight [g/mol]: 234.38

CAS: 90-39-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.89		Aqueous Solubility Prediction Method
logp	2.345		Crippen Method
mcvol	198.730	ml/mol	McGowan Method
rinpol	1785.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1773.00		NIST Webbook
rinpol	1777.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1785.00		NIST Webbook

rmpol	1830.00	NIST Webbook
rmpol	1810.00	NIST Webbook
rmpol	1790.00	NIST Webbook
rmpol	1785.00	NIST Webbook
rmpol	1785.00	NIST Webbook
rmpol	1780.00	NIST Webbook
rmpol	1780.00	NIST Webbook
rmpol	1785.00	NIST Webbook
rmpol	1785.00	NIST Webbook
rmpol	1785.00	NIST Webbook
rmpol	1785.00	NIST Webbook
rmpol	1790.00	NIST Webbook
rmpol	1801.00	NIST Webbook
rmpol	1795.00	NIST Webbook
rmpol	1790.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C90391&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices

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