Genisteine

Other names:	7,14-Methano-2H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazocine, dodecahydro-, [7S-(7«alpha»,7a«alpha»,14«alpha»,14a«alpha»)]- 11-Isosparteine «alpha»-Isospartein «alpha»-Isosparteine L-«alpha»-Isospartein Isosparteine, «alpha» [7S-(7«alpha»,7a«alpha»,14«alpha»,14a«alpha»)]-dodecahydro-7,14-methano-2H,6H-di
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-LXTVHRRPSA-N
Formula:	C15H26N2
SMILES:	C1CCN2CC3CC(CN4CCCCC34)C2C1
Mol. weight [g/mol]:	234.38
CAS:	446-95-7

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	1758.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1701.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1712.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1701.00		NIST Webbook

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=C446957&Units=SI

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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