Aphylline

Other names:	7,14-Methano-2H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazocin-6-one, dodecahydro-, [7R-(7«alpha»,7a«beta»,14«alpha»,14a«alpha»)]- D-aphylline 10-Oxosparteine (+)-Aphylline
Inchi:	InChI=1S/C15H24N2O/c18-15-12-9-11(13-5-2-4-8-17(13)15)10-16-7-3-1-6-14(12)16/h11
InchiKey:	YQMWQSMYVPLYDI-RFQIPJPRSA-N
Formula:	C15H24N2O
SMILES:	O=C1C2CC(CN3CCCCC23)C2CCCCN12
Mol. weight [g/mol]:	248.36
CAS:	577-37-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	1.872		Crippen Method
mcvol	200.300	ml/mol	McGowan Method
rinpol	2165.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2163.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2196.00		NIST Webbook
rinpol	2178.00		NIST Webbook
rinpol	2180.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C577377&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices