

Anagyrine

Other names:

7,14-Methano-4H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazocin-4-one,
Rhombinine

Anagyrin

Monolupin

Monolupine

Rhombinin

Inchi: InChI=1S/C15H20N2O/c18-15-6-3-5-14-11-8-12(10-17(14)15)13-4-1-2-7-16(13)9-11/h3,5

InchiKey: FQEQMASDZFXSJI-FRRDWIJNSA-N

Formula: C15H20N2O

SMILES: O=c1cccc2n1CC1CC2CN2CCCCC12

Mol. weight [g/mol]: 244.33

CAS: 486-89-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.820		Crippen Method
mcvol	191.700	ml/mol	McGowan Method
rinpol	2408.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2387.00		NIST Webbook
rinpol	2375.00		NIST Webbook
rinpol	2375.00		NIST Webbook
rinpol	2406.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2375.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2382.00		NIST Webbook
rinpol	2375.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2390.00		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=C486895&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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