

1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, decahydro-4-(2-propenyl)-, [1S-(1«alpha»,4«alpha»,5«alpha»,11a«alpha»)]-

Other names:

Angustifoline

Jamaicensine

InchiKey: VTIPBIDDZPDAV-UHFFFAOYSA-N

Formula: C₁₄H₂₂N₂O

SMILES: C=CCC1NCC2CC1CN1C(=O)CCCC21

Mol. weight [g/mol]: 234.34

CAS: 550-43-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	1.551		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
rinpol	2080.00		NIST Webbook
rinpol	2083.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2083.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2104.00		NIST Webbook
rinpol	2083.00		NIST Webbook
rinpol	2083.00		NIST Webbook
rinpol	2085.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2083.00		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	2080.00		NIST Webbook

Sources

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>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C550436&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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