

1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, 3-(3-butenyl)-1,2,3,4,5,6-hexahydro-, (1R)-

Other names:

Rhombifoline
Rhombifolin

Inchi: 1,5-Methano-8H-pyrido[1,2-a][1,5]diazocin-8-one, 3-(3-butenyl)-1,2,3,4,5,6-hexahydro-, (1R-cis)
InchiKey: ZVTFRRVBMAUIQW-UHFFFAOYSA-N
Formula: C₁₅H₂₀N₂O
SMILES: C=CCCN1CC2CC(C1)c1cccc(=O)n1C2
Mol. weight [g/mol]: 244.33
CAS: 529-78-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	1.844		Crippen Method
mcvol	198.260	ml/mol	McGowan Method
rinpol	2155.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2160.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2155.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C529782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
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
rinpola:	Non-polar retention indices

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