

2,6-Methano-1,4(2h)-benzoxazocin, 4(3h)-cyclopropyl-6(5h)-phenyl-

Inchi:	InChI=1S/C20H21NO/c1-2-6-15(7-3-1)20-12-17(13-21(14-20)16-10-11-16)22-19-9-5-4-8
InchiKey:	DSCZWDVVVGJVPOP-UHFFFAOYSA-N
Formula:	C20H21NO
SMILES:	c1ccc(C23CC(CN(C4CC4)C2)Oc2ccccc23)cc1
Mol. weight [g/mol]:	291.39
CAS:	99926-14-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.36		Crippen Method
logp	3.602		Crippen Method
mcvol	228.410	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C99926144&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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