

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

Inchi:	InChI=1S/C23H25NO2/c25-22-23(17-9-3-1-4-10-17)15-19(26-21-14-8-7-13-20(21)23)16
InchiKey:	UWOMNSAPCNHFGY-UHFFFAOYSA-N
Formula:	C23H25NO2
SMILES:	O=C1N(C2CCCCC2)CC2CC1(c1ccccc1)c1ccccc1O2
Mol. weight [g/mol]:	347.45
CAS:	101501-17-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.39		Crippen Method
logp	4.299		Crippen Method
mcvol	272.250	ml/mol	McGowan Method

Sources

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=C101501171&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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