

(E)-N-Acetylanhydronarceine

Inchi: InChI=1S/C23H23NO8/c1-12(25)24-8-7-14-10-17-21(32-11-31-17)22(30-4)18(14)15(24)3
InchiKey: ZBARHYHPRYXSAN-OQLLNIDSSA-N
Formula: C23H23NO8
SMILES: COc1ccc(C=C2c3c(cc4c(c3OC)OCO4)CCN2C(C)=O)c(C(=O)O)c1OC
Mol. weight [g/mol]: 441.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.08		Crippen Method
logp	3.042		Crippen Method
mcvol	309.730	ml/mol	McGowan Method
rinpol	3757.00		NIST Webbook
rinpol	3757.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R330822&Units=SI>
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>

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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<https://www.chemeo.com/cid/33-251-6/E-N-Acetylanhydronarceine.pdf>

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