

6-O,N-DiacetylNorcodeine

Inchi:	InChI=1S/C21H23NO5/c1-11(23)22-9-8-21-14-5-7-17(26-12(2)24)20(21)27-19-16(25-3)6
InchiKey:	YJXIDUJUPPLLIM-OBEIKJNWSA-N
Formula:	C21H23NO5
SMILES:	COc1ccc2c3c1OC1C(OC(C)=O)C=CC4C(C2)N(C(C)=O)CCC341
Mol. weight [g/mol]:	369.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	1.989		Crippen Method
mcvol	265.980	ml/mol	McGowan Method
rinpol	2977.00		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=R330817&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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