Morphinan-3,6-«alpha»-diol, 7,8-didehydro-4,5-«alpha»-epoxy-17-methyl-, acetate

Other names: 3-Monoacetylmorphine
Morphine, 3-acetyl

Inchi: InChI=1S/C19H21NO4/c1-10(21)23-15-6-3-11-9-13-12-4-5-14(22)18-19(12,7-8-20(13)2)1

InchiKey: GMLREHXYJDLZOU-ANCOBHAESA-N

Formula: C19H21NO4

SMILES: CC(=O)Oc1ccc2c3c1OC1C(O)C=CC4C(C2)N(C)CCC341

Mol. weight [g/mol]: 327.37

CAS: 29593-26-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	1.418		Crippen Method
mcvol	236.230	ml/mol	McGowan Method
rinpol	2490.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2491.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2491.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29593268&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