

Morphine-3-acetate

Other names:	O3-Monoacetylmorphine O3-MAM
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)
InchiKey:	GMLREHXYJDLZOU-UHFFFAOYSA-N
Formula:	C19H21NO4
SMILES:	CC(=O)Oc1ccc2c3c1OC1C(O)C=CC4C(C2)N(C)CCC341
Mol. weight [g/mol]:	327.37
CAS:	5140-28-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	1.418		Crippen Method
mcvol	236.230	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5140283&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/36-928-2/Morphine-3-acetate.pdf>

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