6-Monoacetylmorphine

Other names:	Morphinan-3,6-«alpha»-diol, 7,8-didehydro-4,5-«alpha»-epoxy-17-methyl-, 6-acetate 6-Acetylmorphine 6-O-Acetylmorphine Monoacetylmorphine Morphine 6-acetate O6 Monoacetylmorphine 6-O-Monoacetylmorphine Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-methyl-, (5«alpha»,6«alpha»)-, 6-acetate 7,8-Didehydro-4,5«alpha»-epoxy-17-methylmorphinan-3,6«alpha»-diol 6-acetate 6-MAM Morphine, a-monoacetyl- CAS# 59833-14-6
Inchi:	InChI=1S/C19H21NO4/c1-10(21)23-15-6-4-12-13-9-11-3-5-14(22)17-16(11)19(12,18(15)
InchiKey:	JJGYGPZNTOPXGV-UHFFFAOYSA-N
Formula:	C19H21NO4
SMILES:	CC(=O)OC1C=CC2C3Cc4ccc(O)c5c4C2(CCN3C)C1O5
Mol. weight [g/mol]:	327.37
CAS:	2784-73-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	1.769		Crippen Method
mcvol	236.230	ml/mol	McGowan Method
rinpol	2493.00		NIST Webbook
rinpol	2608.20		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2537.00		NIST Webbook
rinpol	2537.00		NIST Webbook
rinpol	2495.00		NIST Webbook
rinpol	2552.00		NIST Webbook
rinpol	2535.00		NIST Webbook
rinpol	2517.00		NIST Webbook
rinpol	2537.00		NIST Webbook
rinpol	2608.20		NIST Webbook
rinpol	2535.00		NIST Webbook
rinpol	2493.00		NIST Webbook

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=C2784738&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