6-acetyl-3-propionyl-morphine

Other names:	Morphine, 6-acetyl, propionyl
	Morphine, 6-acetyl, propanoate
	6-monoacetylmorphine, propionic ester
Inchi:	InChI=1S/C22H25NO5/c1-4-18(25)27-16-7-5-13-11-15-14-6-8-17(26-12(2)24)21-22(14,9
InchiKey:	VUBQOPKPSZAJBL-NTUQYPTQSA-N
Formula:	C22H25NO5
SMILES:	CCC(=O)Oc1ccc2c3c1OC1C(OC(C)=O)C=CC4C(C2)N(C)CCC341
Mol. weight [g/mol]:	383.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.91		Crippen Method
logp	2.379		Crippen Method
mcvol	280.070	ml/mol	McGowan Method
rinpol	2722.00		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=R90000&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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