

3-propionyl-morphine

Inchi: InChI=1S/C20H23NO4/c1-3-16(23)24-15-7-4-11-10-13-12-5-6-14(22)19-20(12,8-9-21(13)
InchiKey: LSYABJYKSBROSB-HAGXQDFKSA-N
Formula: C20H23NO4
SMILES: CCC(=O)Oc1ccc2c3c1OC1C(O)C=CC4C(C2)N(C)CCC341
Mol. weight [g/mol]: 341.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.47		Crippen Method
logp	1.808		Crippen Method
mcvol	250.320	ml/mol	McGowan Method
rinsol	2609.00		NIST Webbook

Sources

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=R246554&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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<https://www.chemeo.com/cid/64-737-3/3-propionyl-morphine.pdf>

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