DIHYDROMORPHINONE ACETATE

Other names: 3-Acetylhydromorphone
Hydromorphone, 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)
InchiKey: QVIUKMVKLLVCDU-UHFFFAOYSA-N
Formula: C19H21NO4
SMILES: CC(=O)Oc1ccc2c3c1OC1C(=O)CCC4C(C2)N(C)CCC314
Mol. weight [g/mol]: 327.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Cheméo Relay (1.0)
logp	1.850		Crippen Method
mcvol	236.230	ml/mol	McGowan Method
tf	425.38	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C14696221&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point