

Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-methyl- (5«alpha»,6«alpha»)-, bis(trifluoroacetate) (ester)

Other names:

Morphine bis-TFA
Morphine, O,O-bis-TFA

Morphine O,O-bis(trifluoroacetate)

Morphine, TFA

Inchi: InChI=1S/C21H17F6NO5/c1-28-7-6-19-10-3-5-13(32-18(30)21(25,26)27)16(19)33-15-12
InchiKey: BTEJWQJJORMUAG-UHFFFAOYSA-N
Formula: C21H17F6NO5
SMILES: CN1CCC23c4c5ccc(OC(=O)C(F)(F)F)c4OC2C(OC(=O)C(F)(F)F)C=CC3C1C5
Mol. weight [g/mol]: 477.35
CAS: 66091-22-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.82		Crippen Method
logp	3.073		Crippen Method
mcvol	276.600	ml/mol	McGowan Method

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C66091223&Units=SI>

Legend

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

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