

Atropine formate

Inchi: InChI=1S/C18H23NO4/c1-19-14-7-8-15(19)10-16(9-14)23-18(21)17(11-22-12-20)13-5-3
InchiKey: ZJENKMNPPJTIBO-UHFFFAOYSA-N
Formula: C18H23NO4
SMILES: CN1C2CCC1CC(OC(=O)C(COC=O)c1cccc1)C2
Mol. weight [g/mol]: 317.38
CAS: 645419-61-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	2.112		Crippen Method
mcvol	243.860	ml/mol	McGowan Method
rinpol	2312.70		NIST Webbook
rinpol	2312.70		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C645419610&Units=SI>
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>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/99-454-9/Atropine-formate.pdf>

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