

Morclofone

Inchi: InChI=1S/C21H24ClNO5/c1-25-18-13-16(20(24)15-3-5-17(22)6-4-15)14-19(26-2)21(18)2
InchiKey: KVCJCEKJKGLBOK-UHFFFAOYSA-N
Formula: C21H24ClNO5
SMILES: COc1cc(C(=O)c2ccc(Cl)cc2)cc(OC)c1OCCN1CCOCC1
Mol. weight [g/mol]: 405.87
CAS: 31848-01-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.12		Crippen Method
logp	3.299		Crippen Method
mcvol	295.640	ml/mol	McGowan Method
rinpole	3101.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C31848018&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/21-885-6/Morclofone.pdf>

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