

Tropine, trifluoroacetate

Inchi: InChI=1S/C10H14F3NO2/c1-14-6-2-3-7(14)5-8(4-6)16-9(15)10(11,12)13/h6-8H,2-5H2,1H
InchiKey: FIHZLPJYASPHBR-UHFFFAOYSA-N
Formula: C10H14F3NO2
SMILES: CN1C2CCC1CC(OC(=O)C(F)(F)F)C2
Mol. weight [g/mol]: 237.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.23		Crippen Method
logp	1.717		Crippen Method
mcvol	152.770	ml/mol	McGowan Method
rinpole	1213.00		NIST Webbook
rinpole	1213.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375738&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/113-333-6/Tropine-trifluoroacetate.pdf>

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