Tropine, heptafluorobutyrate

Inchi: InChI=1S/C12H14F7NO2/c1-20-6-2-3-7(20)5-8(4-6)22-9(21)10(13,14)11(15,16)12(17,18
InchiKey: HPUURXJBHKUNTM-UHFFFAOYSA-N
Formula: C12H14F7NO2
SMILES: CN1C2CCC1CC(OC(=O)C(F)(F)C(F)(F)C(F)(F)F)C2
Mol. weight [g/mol]: 337.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	2.988		Crippen Method
mcvol	188.030	ml/mol	McGowan Method
rinpol	1287.00		NIST Webbook
rinpol	1287.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375736&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
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.