Imidazole, 1-[1-(4-chloro-2-trifluoromethylphenylimino)-2-pro

Inchi: InChI=1S/C14H13ClF3N3O/c1-2-7-22-13(21-6-5-19-9-21)20-12-4-3-10(15)8-11(12)14(16

InchiKey: ICPXOBRVTVXPQP-UHFFFAOYSA-N

Formula: C14H13ClF3N3O

SMILES: CCCOC(=Nc1ccc(Cl)cc1C(F)(F)F)n1ccnc1

Mol. weight [g/mol]: 331.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.19		Crippen Method
logp	4.518		Crippen Method
mcvol	213.960	ml/mol	McGowan Method
rinpol	2117.00		NIST Webbook
rinpol	2117.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=R537563&Units=SI

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.