4-Chloro-7-(trifluoromethyl)quinoline

Other names: Quinoline, 4-chloro-7-(trifluoromethyl)-
Inchi: InChI=1S/C10H5ClF3N/c11-8-3-4-15-9-5-6(10(12,13)14)1-2-7(8)9/h1-5H
InchiKey: LLRQVSZVVAKRJA-UHFFFAOYSA-N
Formula: C10H5ClF3N
SMILES: FC(F)(F)c1ccc2c(Cl)ccnc2c1
Mol. weight [g/mol]: 231.60
CAS: 346-55-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.907		Crippen Method
mcvol	136.070	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C346554&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