

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

Latest version available from:

<https://www.chemeo.com/cid/28-446-6/4-Chloro-7-trifluoromethyl-quinoline.pdf>

Generated by Cheméo on 2024-04-26 03:40:15.098681556 +0000 UTC m=+16392064.019258883.

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