2-CHLORO-4-TRIFLUOROMETHYLPYRIDINE

Other names: Pyridine, 2-chloro-4-(trifluoromethyl)-
Inchi: InChI=1S/C6H3ClF3N/c7-5-3-4(1-2-11-5)6(8,9)10/h1-3H
InchiKey: GBNPVXZNWBWNEN-UHFFFAOYSA-N
Formula: C6H3ClF3N
SMILES: FC(F)(F)c1ccnc(Cl)c1
Mol. weight [g/mol]: 181.54

Physical Properties

Property code	Value	Unit	Source
ie	10.25	eV	Cheméo Relay (1.0)
logp	2.754		Crippen Method
mcvol	99.170	ml/mol	McGowan Method
tb	423.07	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C81565186&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

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