

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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<https://www.chemeo.com/cid/91-839-0/2-CHLORO-4-TRIFLUOROMETHYLPYRIDINE.pdf>

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