2-TRIFLUOROMETHYL-5-METHOXYBENZIMIDAZ

Other names: Benzimidazole, 5-methoxy-2-(trifluoromethyl)-
Inchi: InChI=1S/C9H7F3N2O/c1-15-5-2-3-6-7(4-5)14-8(13-6)9(10,11)12/h2-4H,1H3,(H,13,14)
InchiKey: GPYQJBAVCKSQTJ-UHFFFAOYSA-N
Formula: C9H7F3N2O
SMILES: COc1ccc2[nH]c(C(F)(F)F)nc2c1
Mol. weight [g/mol]: 216.16

Physical Properties

Property code	Value	Unit	Source
logp	2.108		Crippen Method
mcvol	129.890	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3671656&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

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume