

2-TRIFLUOROMETHYL-5-METHOXYBENZIMIDAZOLE

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:	GPYQJBAVCKSQJTJ-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

Latest version available from:

<https://www.chemeo.com/cid/48-496-9/2-TRIFLUOROMETHYL-5-METHOXYBENZIMIDAZOLE.pdf>

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