

Benzimidazole, 4-bromo-6-nitro-2-(trifluoromethyl)-

Inchi:	InChI=1S/C8H3BrF3N3O2/c9-4-1-3(15(16)17)2-5-6(4)14-7(13-5)8(10,11)12/h1-2H,(H,13
InchiKey:	RJHWHAVCPNBCTM-UHFFFAOYSA-N
Formula:	C8H3BrF3N3O2
SMILES:	O=[N+]([O-])c1cc(Br)c2nc(C(F)(F)F)[nH]c2c1
Mol. weight [g/mol]:	310.03
CAS:	6609-37-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.18		Crippen Method
logp	2.771		Crippen Method
mcvol	144.850	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6609376&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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