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

Inchi: InChI=1S/C8H3BrF3N3O2/c9-3-1-4-6(5(2-3)15(16)17)14-7(13-4)8(10,11)12/h1-2H,(H,13

InchiKey: USUPLSWSXSTERT-UHFFFAOYSA-N

Formula: C8H3BrF3N3O2

SMILES: O=[N+]([O-])c1cc(Br)cc2[nH]c(C(F)(F)F)nc12

Mol. weight [g/mol]: 310.03

CAS: 6609-36-5

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/ci990307l

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=C6609365&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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