

Benzimidazole, 5,6-dinitro-2-(trifluoromethyl)-

Inchi:	InChI=1S/C8H3F3N4O4/c9-8(10,11)7-12-3-1-5(14(16)17)6(15(18)19)2-4(3)13-7/h1-2H,(H
InchiKey:	OOJCWFWANPATNU-UHFFFAOYSA-N
Formula:	C8H3F3N4O4
SMILES:	O=[N+]([O-])c1cc2nc(C(F)(F)F)[nH]c2cc1[N+](=O)[O-]
Mol. weight [g/mol]:	276.13
CAS:	2338-24-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.67		Crippen Method
logp	1.916		Crippen Method
mcvol	144.770	ml/mol	McGowan Method

Sources

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=C2338241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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<https://www.chemeo.com/cid/38-148-6/Benzimidazole-5-6-dinitro-2-trifluoromethyl.pdf>

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