

# Benzimidazole, 5-nitro-2-(trifluoromethyl)-

<b>Inchi:</b>	InChI=1S/C8H4F3N3O2/c9-8(10,11)7-12-5-2-1-4(14(15)16)3-6(5)13-7/h1-3H,(H,12,13)
<b>InchiKey:</b>	FEJRBJIEEALTTL-UHFFFAOYSA-N
<b>Formula:</b>	C8H4F3N3O2
<b>SMILES:</b>	O=[N+]([O-])c1ccc2[nH]c(C(F)(F)F)nc2c1
<b>Mol. weight [g/mol]:</b>	231.13
<b>CAS:</b>	327-19-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	2.008		Crippen Method
mcvol	127.350	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C327195&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C327195&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/39-119-7/Benzimidazole-5-nitro-2-trifluoromethyl.pdf>

Generated by Cheméo on 2024-04-19 02:10:11.558801345 +0000 UTC m=+15781860.479378661.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.