

Etisazole

Inchi:	InChI=1S/C9H10N2S/c1-2-10-9-7-5-3-4-6-8(7)12-11-9/h3-6H,2H2,1H3,(H,10,11)
InchiKey:	CPYSWRYVVSINXMC-UHFFFAOYSA-N
Formula:	C9H10N2S
SMILES:	CCNc1nsc2ccccc12
Mol. weight [g/mol]:	178.25
CAS:	7716-60-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	2.728		Crippen Method
mcvol	135.060	ml/mol	McGowan Method
rinpol	1668.00		NIST Webbook
rinpol	1668.00		NIST Webbook

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=C7716601&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/24-245-3/Etisazole.pdf>

Generated by Cheméo on 2025-12-05 20:15:18.214671771 +0000 UTC m=+4713915.744712434.

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