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: CPYSWRYVSINXMC-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