1,2-Benzisothiazole

Other names:	Benzo[d]isothiazole
	1-Thia-2-azaindene
	Benzisothiazole-1,2
	1,2-benzothiazole
	benzisothiazole
Inchi:	InChI=1S/C7H5NS/c1-2-4-7-6(3-1)5-8-9-7/h1-5H
InchiKey:	CSNIZNHTOVFARY-UHFFFAOYSA-N
Formula:	C7H5NS
SMILES:	c1ccc2sncc2c1
Mol. weight [g/mol]:	135.19
CAS:	272-16-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	2.296		Crippen Method
mcvol	96.900	ml/mol	McGowan Method
rinpol	1221.00		NIST Webbook
ripol	1955.00		NIST Webbook
ripol	1955.00		NIST Webbook

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=C272162&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices