1,2-benzisothiazol-3(2H)-one

Inchi: InChI=1S/C7H5NOS/c9-7-5-3-1-2-4-6(5)10-8-7/h1-4H,(H,8,9)
InchiKey: DMSMPAJRVJJAGA-UHFFFAOYSA-N
Formula: C7H5NOS
SMILES: O=c1[nH]sc2ccccc12
Mol. weight [g/mol]: 151.19

Physical Properties

Property code	Value	Unit	Source
hfus	20.87	kJ/mol	Combined experimental and computational study on the energetics of 1,2-benzisothiazol-3(2H)-one and 1,4-benzothiazin-3(2H, 4H)-one
hfus	112.40	kJ/mol	Combined experimental and computational study on the energetics of 1,2-benzisothiazol-3(2H)-one and 1,4-benzothiazin-3(2H, 4H)-one
log10ws	-1.67		Crippen Method
logp	1.108		Crippen Method
mcvol	102.770	ml/mol	McGowan Method
tf	428.79	K	Combined experimental and computational study on the energetics of 1,2-benzisothiazol-3(2H)-one and 1,4-benzothiazin-3(2H, 4H)-one

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Combined experimental and computational study on the energetics of 1,2-benzisothiazol-3(2H)-one and 1,4-benzothiazin-3(2H, 4H)-one: https://www.doi.org/10.1016/j.jct.2010.11.006

Legend

hfus:	Enthalpy of fusion at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point