Benzothiazol-2-ylacetonitrile

Other names: Benzothiazol-2-ylacetonitrile
Inchi: InChI=1S/C9H6N2S/c10-6-5-9-11-7-3-1-2-4-8(7)12-9/h1-4H,5H2
InchiKey: ZMZSYUSDGRJZNT-UHFFFAOYSA-N
Formula: C9H6N2S
SMILES: N#CCc1nc2ccccc2s1
Mol. weight [g/mol]: 174.23

Physical Properties

Property code	Value	Unit	Source
ie	9.01	eV	Cheméo Relay (1.0)
log10ws	-2.48		Cheméo Relay (1.0)
logp	2.362		Crippen Method
mcvol	126.460	ml/mol	McGowan Method
tb	590.35	K	Cheméo Relay (1.0)
tf	395.14	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56278503&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point