methabenzthiazuron

Inchi: InChI=1S/C10H11N3OS/c1-11-9(14)13(2)10-12-7-5-3-4-6-8(7)15-10/h3-6H,1-2H3,(H,11,
InchiKey: RRVIAQKBTUQODI-UHFFFAOYSA-N
Formula: C10H11N3OS
SMILES: CNC(=O)N(C)c1nc2ccccc2s1
Mol. weight [g/mol]: 221.29

Physical Properties

Property code	Value	Unit	Source
ie	8.38	eV	Cheméo Relay (1.0)
logp	2.072		Crippen Method
mcvol	160.700	ml/mol	McGowan Method
tb	601.11	K	Cheméo Relay (1.0)
tf	431.16	K	Cheméo Relay (1.0)

Sources

Octanol/Water Partition Coefficient of Selected Herbicides: Determination Using Shake-Flask Method and Reversed-Phase High-Performance Liquid Chromatography: https://www.doi.org/10.1021/je049947x
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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point