

2-(2-Thiazolylazo)-p-cresol

Inchi: InChI=1S/C10H9N3OS/c1-7-2-3-9(14)8(6-7)12-13-10-11-4-5-15-10/h2-6,14H,1H3
InchiKey: MZRKINSTWYZJLV-UHFFFAOYSA-N
Formula: C10H9N3OS
SMILES: Cc1ccc(O)c(N=Nc2nccs2)c1
Mol. weight [g/mol]: 219.27

Physical Properties

Property code	Value	Unit	Source
ie	8.11	eV	Cheméo Relay (1.0)
logp	3.573		Crippen Method
mcvol	156.400	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1823445&Units=SI>

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

Legend

ie: Ionization energy
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/33-269-7/2-2-Thiazolylazo-p-cresol.pdf>

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