

Pyrazine, phenylthio

Other names: (Phenylthio)pyrazine
Inchi: InChI=1S/C10H8N2S/c1-2-4-9(5-3-1)13-10-8-11-6-7-12-10/h1-8H
InchiKey: VAUCOCSGTRUZW-UHFFFAOYSA-N
Formula: C10H8N2S
SMILES: c1ccc(Sc2cnccn2)cc1
Mol. weight [g/mol]: 188.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.42		Crippen Method
logp	2.628		Crippen Method
mcvol	140.550	ml/mol	McGowan Method
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook
ripol	2400.00		NIST Webbook
ripol	2400.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R36412&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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

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