

[1,2,4]Triazolo[1,5-a]pyrazine

Other names: s-Triazolo[1,5-a]pyrazine
Inchi: InChI=1S/C5H4N4/c1-2-9-5(3-6-1)7-4-8-9/h1-4H
InchiKey: DFDJVPRVKHSWQH-UHFFFAOYSA-N
Formula: C5H4N4
SMILES: c1cn2ncnc2cn1
Mol. weight [g/mol]: 120.11
CAS: 399-66-6

Physical Properties

Property code	Value	Unit	Source
ie	9.60	eV	NIST Webbook
log10ws	-1.73		Crippen Method
logp	0.124		Crippen Method
mcvol	82.310	ml/mol	McGowan Method
ripol	1675.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C399666&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/23-125-7/1-2-4-Triazolo-1-5-a-pyrazine.pdf>

Generated by Cheméo on 2024-05-02 14:33:42.924577012 +0000 UTC m=+16949671.845154324.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.