

4-Cl-pyrazole

Inchi: InChI=1S/C3H3ClN2/c4-3-1-5-2-6-3/h1-2H,(H,5,6)
InchiKey: BQRBAXFOPZRMCU-UHFFFAOYSA-N
Formula: C3H3ClN2
SMILES: Clc1cnc[nH]1
Mol. weight [g/mol]: 102.52
CAS: 15965-31-8

Physical Properties

Property code	Value	Unit	Source
affp	868.50	kJ/mol	NIST Webbook
basg	834.90	kJ/mol	NIST Webbook
log10ws	-1.14		Crippen Method
logp	0.581		Crippen Method
mcvol	65.870	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C15965318&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

affp: Proton affinity
basg: Gas basicity
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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