

Pyrazole, 4-iodo

Inchi: InChI=1S/C3H3IN2/c4-3-1-5-6-2-3/h1-2H,(H,5,6)
InchiKey: LLNQWPTUJJYTTE-UHFFFAOYSA-N
Formula: C3H3IN2
SMILES: Ic1cn[nH]c1
Mol. weight [g/mol]: 193.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.60		Crippen Method
logp	0.532		Crippen Method
mcvol	79.450	ml/mol	McGowan Method
rinpol	1220.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R43926&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/51-046-4/Pyrazole-4-iodo.pdf>

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