

Indolizine

Other names:	Pyrrolo[1,2-a]pyridine Indolizin Pyrrocolin Pyrrocoline
Inchi:	InChI=1S/C8H7N/c1-2-6-9-7-3-5-8(9)4-1/h1-7H
InchiKey:	HOBCFUWDNJPFB-UHFFFAOYSA-N
Formula:	C8H7N
SMILES:	c1ccn2cccc2c1
Mol. weight [g/mol]:	117.15
CAS:	274-40-8

Physical Properties

Property code	Value	Unit	Source
ie	7.24	eV	NIST Webbook
ie	7.24	eV	NIST Webbook
ie	7.26	eV	NIST Webbook
log10ws	-2.43		Crippen Method
logp	1.939		Crippen Method
mvol	94.640	ml/mol	McGowan Method
tb	478.20	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C274408&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
mcpvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature

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