

Quinazoline, 4-methyl-

Other names:	4-Methylquinazoline
Inchi:	InChI=1S/C9H8N2/c1-7-8-4-2-3-5-9(8)11-6-10-7/h2-6H,1H3
InchiKey:	JWEOEZZCZCCPJL-UHFFFAOYSA-N
Formula:	C9H8N2
SMILES:	Cc1ncnc2ccccc12
Mol. weight [g/mol]:	144.17
CAS:	700-46-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	1.938		Crippen Method
mcvol	114.410	ml/mol	McGowan Method
rinpol	1364.00		NIST Webbook
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rinpol	1364.00		NIST Webbook

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=C700469&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

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