

8-Quinolinemethanethiol

Inchi:	InChI=1S/C10H9NS/c12-7-9-4-1-3-8-5-2-6-11-10(8)9/h1-6,12H,7H2
InchiKey:	FINMYCNANOBTK-UHFFFAOYSA-N
Formula:	C10H9NS
SMILES:	SCc1cccc2cccnc12
Mol. weight [g/mol]:	175.25
CAS:	103264-35-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.665		Crippen Method
mcvol	134.870	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103264353&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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