

Quinoline, 8,8'-(ethylenediimino)di-

Inchi:	InChI=1S/C20H18N4/c1-5-15-7-3-11-23-19(15)17(9-1)21-13-14-22-18-10-2-6-16-8-4-12-
InchiKey:	XJCUTXHPPQVIBV-UHFFFAOYSA-N
Formula:	C20H18N4
SMILES:	c1cnc2c(NCCNc3cccc4ccnc34)cccc2c1
Mol. weight [g/mol]:	314.38
CAS:	67201-67-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.28		Crippen Method
logp	4.307		Crippen Method
mcvol	246.140	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67201676&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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