

[1,2,4]Triazolo[4,3-a]quinoline

Other names:	2,3,9b-Triazabenz[e]indene 2,3,9b-Triazabenz[g]indene s-Triazolo[4,3-a]quinoline Triazolo(4,3a)quinoline
Inchi:	InChI=1S/C10H7N3/c1-2-4-9-8(3-1)5-6-10-12-11-7-13(9)10/h1-7H
InchiKey:	PIRYKGLQLCKQPG-UHFFFAOYSA-N
Formula:	C10H7N3
SMILES:	<chem>c1ccc2c(c1)ccc1nncn12</chem>
Mol. weight [g/mol]:	169.18
CAS:	235-06-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	1.883		Crippen Method
mcvol	123.320	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=C235063&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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