

as-Triazino[6,5-c]quinoline, 2-methylamino-

Other names:	2-Methylamino-as-triazino(6,5-c)quinoline
Inchi:	InChI=1S/C11H9N5/c1-12-11-14-10-7-4-2-3-5-8(7)13-6-9(10)15-16-11/h2-6H,1H3,(H,12,
InchiKey:	IJHKEEBMQBKHPU-UHFFFAOYSA-N
Formula:	C11H9N5
SMILES:	CN=c1nnc2cnc3ccccc3c2[nH]1
Mol. weight [g/mol]:	211.22
CAS:	81547-13-9

Physical Properties

Property code	Value	Unit	Source
ie	8.47 ± 0.10	eV	NIST Webbook
log10ws	-3.26		Crippen Method
logp	0.555		Crippen Method
mcvol	153.070	ml/mol	McGowan Method

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=C81547139&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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