

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

Other names:	2-Amino-as-triazino(6,5-c)-quinoline
Inchi:	InChI=1S/C10H7N5/c11-10-13-9-6-3-1-2-4-7(6)12-5-8(9)14-15-10/h1-5H,(H2,11,13,15)
InchiKey:	QKQLJPYBCAVMIU-UHFFFAOYSA-N
Formula:	C10H7N5
SMILES:	<chem>N=c1nnc2cnc3ccccc3c2[nH]1</chem>
Mol. weight [g/mol]:	197.20
CAS:	51294-37-2

Physical Properties

Property code	Value	Unit	Source
ie	8.58 ± 0.10	eV	NIST Webbook
log10ws	-4.59		Crippen Method
logp	0.504		Crippen Method
mcvol	138.980	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=C51294372&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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