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

Other names: 2-Dimethylamino-as-triazino(6,5-c)quinoline
Inchi: InChI=1S/C12H11N5/c1-17(2)12-14-11-8-5-3-4-6-9(8)13-7-10(11)15-16-12/h3-7H,1-2H3
InchiKey: ZRJVJFSBPZFDFL-UHFFFAOYSA-N
Formula: C12H11N5
SMILES: CN(C)c1nnc2cnc3ccccc3c2n1
Mol. weight [g/mol]: 225.25
CAS: 81547-14-0

Physical Properties

Property code	Value	Unit	Source
ie	8.15 ± 0.10	eV	NIST Webbook
log10ws	-4.05		Crippen Method
logp	1.639		Crippen Method
mcvol	167.160	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C81547140&Units=SI

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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