

Proflavine

Other names:	3,6-Acridinediamine Acridine, 3,6-diamino- 3,6-Diaminoacridine 2,8-Diaminoacridinium 3,6-Diaminoacridinium Isoflav base Proflavin Profura Progarmed 3,7-Diamino-5-azaanthracene
Inchi:	InChI=1S/C13H11N3/c14-10-3-1-8-5-9-2-4-11(15)7-13(9)16-12(8)6-10/h1-7H,14-15H2
InchiKey:	WDVSHHCDHLJJJR-UHFFFAOYSA-N
Formula:	C13H11N3
SMILES:	<chem>Nc1ccc2cc3ccc(N)cc3nc2c1</chem>
Mol. weight [g/mol]:	209.25
CAS:	92-62-6

Physical Properties

Property code	Value	Unit	Source
chs	-6711.00 ± 13.00	kJ/mol	NIST Webbook
log10ws	-4.11		Crippen Method
logp	2.552		Crippen Method
mcvol	161.290	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C92626&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/83-111-6/Proflavine.pdf>

Generated by Cheméo on 2024-04-24 16:12:34.980212506 +0000 UTC m=+16264403.900789817.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.