

9-Acridinamine

Other names:	Acridine, 9-amino- Aminacrin Aminacrine Izoacridina Monacrin 10-Amino-5-azaanthracene 9-Aminoacridine 9AA Aminoacridine 9-Aminoakridin Acridin-9-amine NSC 13000
Inchi:	InChI=1S/C13H10N2/c14-13-9-5-1-3-7-11(9)15-12-8-4-2-6-10(12)13/h1-8H,(H2,14,15)
InchiKey:	XJGFWWJLMVZSIG-UHFFFAOYSA-N
Formula:	C13H10N2
SMILES:	Nc1c2ccccc2nc2ccccc12
Mol. weight [g/mol]:	194.23
CAS:	90-45-9

Physical Properties

Property code	Value	Unit	Source
chs	-6704.00 ± 7.10	kJ/mol	NIST Webbook
log10ws	-4.48		Crippen Method
logp	2.970		Crippen Method
mcvol	151.310	ml/mol	McGowan Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	115.00	kJ/mol	520.00	NIST Webbook

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=C90459&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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