

9(10H)-Acridinone, 10-methyl-

Other names:	10-Methyl-9(10H)-acridone 10-Methyl-9-acridanone 10-Methylacridon 10-methyl-9(10H)-acridinone 10-methylacridin-9(10H)-one 10-methylacridin-9-one 10-methylacridone 9-Acridanone, 10-methyl- 9-Hydro-10-methyl-9-oxoacridine N-Methylacridone N-methyl-9-acridone
Inchi:	InChI=1S/C14H11NO/c1-15-12-8-4-2-6-10(12)14(16)11-7-3-5-9-13(11)15/h2-9H,1H3
InchiKey:	XUVKSPGPPFPQN-UHFFFAOYSA-N
Formula:	C14H11NO
SMILES:	<chem>Cn1c2ccccc2c(=O)c2ccccc21</chem>
Mol. weight [g/mol]:	209.24
CAS:	719-54-0

Physical Properties

Property code	Value	Unit	Source
ie	7.53 ± 0.02	eV	NIST Webbook
log10ws	-4.46		Aqueous Solubility Prediction Method
logp	2.692		Crippen Method
mcvol	161.290	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	29.70	kJ/mol	479.00	NIST Webbook
hvapt	123.80	kJ/mol	298.15	Experimental and computational thermochemical studies of acridone and N-methylacridone

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C719540&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Experimental and computational thermochemical studies of acridone and N-methylacridone: <https://www.doi.org/10.1016/j.jct.2017.11.002>

Legend

hfust:	Enthalpy of fusion at a given temperature
hvapt:	Enthalpy of vaporization at a given temperature
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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