

9(10H)-Acridinone

Other names:	9(10H)-acridone 9,10-dihydro-9-oxo-acridine 9,10-dihydro-9-oxoacridine 9,l0-Dihydro-9-oxoacridine 9-acridanone 9-acridone CK 103 acridanone acridin-9-one acridine, 9,10-dihydro-9-oxo-acridone
Inchi:	InChI=1S/C13H9NO/c15-13-9-5-1-3-7-11(9)14-12-8-4-2-6-10(12)13/h1-8H,(H,14,15)
InchiKey:	FZEYVTFCMJSGMP-UHFFFAOYSA-N
Formula:	C13H9NO
SMILES:	O=c1c2ccccc2[nH]c2cccc12
Mol. weight [g/mol]:	195.22
CAS:	578-95-0

Physical Properties

Property code	Value	Unit	Source
chs	-6300.30 ± 2.50	kJ/mol	NIST Webbook
hf	34.60 ± 2.60	kJ/mol	NIST Webbook
hfs	-101.60 ± 2.60	kJ/mol	NIST Webbook
hsub	136.15 ± 0.45	kJ/mol	NIST Webbook
hsub	136.20 ± 0.50	kJ/mol	NIST Webbook
ie	7.60 ± 0.03	eV	NIST Webbook
log10ws	-3.72		Crippen Method
logp	2.199		Crippen Method
mcvol	147.200	ml/mol	McGowan Method
rinpol	2362.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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hfust	32.50	kJ/mol	640.00	NIST Webbook
hvapt	133.40	kJ/mol	298.15	Experimental and computational thermochemical studies of acridone and N-methylacridone

Sources

Experimental and computational thermochemical studies of acridone and N-methylacridone:
McGowan Method:

<https://www.doi.org/10.1016/j.jct.2017.11.002>

NIST Webbook:

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

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C578950&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
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
rinpol:	Non-polar retention indices

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