

# Phenyl acridine-9-carboxylate

<b>Inchi:</b>	InChI=1S/C20H13NO2/c22-20(23-14-8-2-1-3-9-14)19-15-10-4-6-12-17(15)21-18-13-7-5-
<b>InchiKey:</b>	QIYUZWMXMSNPRG-UHFFFAOYSA-N
<b>Formula:</b>	C20H13NO2
<b>SMILES:</b>	O=C(Oc1ccccc1)c1c2ccccc2nc2ccccc12
<b>Mol. weight [g/mol]:</b>	299.32
<b>CAS:</b>	109392-90-7

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.93		Crippen Method
logp	4.607		Crippen Method
mcpvol	223.640	ml/mol	McGowan Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	39.20	kJ/mol	464.00	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C109392907&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C109392907&amp;Units=SI</a>

## Legend

**hfust:** Enthalpy of fusion at a given temperature

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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