Benz[c]acridine

Other names:	«alpha»-Chrysidine
	«alpha»-Naphthacridine
	B(c)AC
	12-Azabenz(a)anthracene
	3,4-Benzacridine
	7,8-Benzacridine
	3,4-Benzoacridine
	Rcra waste number U016
	NSC 89261
	Benzo[c]acridine
Inchi:	InChI=1S/C17H11N/c1-3-7-15-12(5-1)9-10-14-11-13-6-2-4-8-16(13)18-17(14)15/h1-11H
InchiKey:	OAPPEBNXKAKQGS-UHFFFAOYSA-N
Formula:	C17H11N
SMILES:	c1ccc2nc3c(ccc4ccccc43)cc2c1
Mol. weight [g/mol]:	229.28
CAS:	225-51-4

Physical Properties

Property code	Value	Unit	Source
ie	8.10 ± 0.10	eV	NIST Webbook
log10ws	-6.65		Crippen Method
logp	4.541		Crippen Method
mcvol	178.230	ml/mol	McGowan Method
rinpol	2444.00		NIST Webbook
rinpol	392.06		NIST Webbook
rinpol	392.11		NIST Webbook
rinpol	392.41		NIST Webbook
rinpol	393.41		NIST Webbook
rinpol	392.60		NIST Webbook
rinpol	392.50		NIST Webbook
rinpol	392.60		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.30	kJ/mol	381.40	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C225514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion 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