Dibenz[a,j]acridine

Other names:	Dibenzo[a,j]acridine
	1,2:7,8-Dibenzacridine
	7-Azadibenz[a,j]anthracene
	1,2,7,8-Dibenzacridine
	Db(a,j)ac
Inchi:	InChI=1S/C21H13N/c1-3-7-16-14(5-1)9-11-20-18(16)13-19-17-8-4-2-6-15(17)10-12-21(1
InchiKey:	ANUCHZVCBDOPOX-UHFFFAOYSA-N
Formula:	C21H13N
SMILES:	c1ccc2c(c1)ccc1nc3ccc4ccccc4c3cc12
Mol. weight [g/mol]:	279.33
CAS:	224-42-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.46		Crippen Method
logp	5.694		Crippen Method
mcvol	215.130	ml/mol	McGowan Method
rinpol	490.53		NIST Webbook
rinpol	485.37		NIST Webbook
rinpol	490.66		NIST Webbook
rinpol	490.66		NIST Webbook
rinpol	3197.00		NIST Webbook
rinpol	487.56		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	25.50	kJ/mol	492.70	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C224420&Units=SI

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
rinpol:	Non-polar retention indices