Dibenz(a,h)acridine

Other names:	7-Azadibenz(a,h)anthracene
	Db(a,h)ac
	Dibenz(a,d)acridine
	1,2,5,6-Dibenzacridine
	1,2,5,6-Dibenzoacridine
Inchi:	InChI=1S/C21H13N/c1-3-7-17-14(5-1)11-12-20-19(17)13-16-10-9-15-6-2-4-8-18(15)21(1
InchiKey:	JNCSIWAONQTVCF-UHFFFAOYSA-N
Formula:	C21H13N
SMILES:	c1ccc2c(c1)ccc1nc3c(ccc4ccccc43)cc12
Mol. weight [g/mol]:	279.33
CAS:	226-36-8

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	3047.00		NIST Webbook
rinpol	488.55		NIST Webbook
rinpol	488.55		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.60	kJ/mol	499.70	NIST Webbook

Sources

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=C226368&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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