Benz(a)acridine, 9,10,12-trimethyl-

Other names:	5,7,8-Trimethyl-3:4-benzacridine
	2,3,10 Trimethyl,5:6 benzacridine
	9,10,12-Trimethylbenz[a]acridine
Inchi:	InChI=1S/C20H17N/c1-12-10-17-14(3)20-16-7-5-4-6-15(16)8-9-18(20)21-19(17)11-13(12
InchiKey:	CWOZJMDRFAMWLF-UHFFFAOYSA-N
Formula:	C20H17N
SMILES:	Cc1cc2nc3ccc4ccccc4c3c(C)c2cc1C
Mol. weight [g/mol]:	271.36
CAS:	63040-02-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.08		Crippen Method
logp	5.466		Crippen Method
mcvol	220.500	ml/mol	McGowan Method
rinpol	466.79		NIST Webbook
rinpol	466.79		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63040028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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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