

(Z) 9-(2[3,5-Dimethylphenyl]ethenyl)acridine

Inchi:	InChI=1S/C23H19N/c1-16-13-17(2)15-18(14-16)11-12-19-20-7-3-5-9-22(20)24-23-10-6-4
InchiKey:	ZUTGIWMIEXMSGV-QXMHVHEDSA-N
Formula:	C23H19N
SMILES:	<chem>Cc1cc(C)cc(C=Cc2c3ccccc3nc3ccccc23)c1</chem>
Mol. weight [g/mol]:	309.40
CAS:	88332-47-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.40		Crippen Method
logp	6.175		Crippen Method
mcvol	254.170	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C88332472&Units=SI

Legend

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

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