

Carbazole, 1,4,8-trimethyl-

Other names:	1,4,8-Trimethylcarbazole
Inchi:	InChI=1S/C15H15N/c1-9-7-8-11(3)15-13(9)12-6-4-5-10(2)14(12)16-15/h4-8,16H,1-3H3
InchiKey:	DKMJSUBUAMUZAJ-UHFFFAOYSA-N
Formula:	C15H15N
SMILES:	<chem>Cc1cccc2c1[nH]c1c(C)ccc(C)c12</chem>
Mol. weight [g/mol]:	209.29
CAS:	78787-83-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.73		Crippen Method
logp	3.764		Crippen Method
mcvol	173.810	ml/mol	McGowan Method
rmpol	1969.00		NIST Webbook
rmpol	1969.00		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=C78787834&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices

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