

Carbazole, 2,6-dimethyl-

Other names:	2,6-Dimethylcarbazole
Inchi:	InChI=1S/C14H13N/c1-9-4-6-13-12(7-9)11-5-3-10(2)8-14(11)15-13/h3-8,15H,1-2H3
InchiKey:	JEQGMFVANDIHGJ-UHFFFAOYSA-N
Formula:	C14H13N
SMILES:	<chem>Cc1ccc2c(c1)[nH]c1ccc(C)cc12</chem>
Mol. weight [g/mol]:	195.26
CAS:	78787-80-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.25		Crippen Method
logp	3.456		Crippen Method
mcvol	159.720	ml/mol	McGowan Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
tf	481.65 ± 2.00	K	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=C78787801&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point

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