

9H-Carbazole, 2-methyl-

Other names:	Carbazole, 2-methyl- 2-Methylcarbazole 2-Methyldibenzopyrrole 2-methyl-9H-carbazole
Inchi:	InChI=1S/C13H11N/c1-9-6-7-11-10-4-2-3-5-12(10)14-13(11)8-9/h2-8,14H,1H3
InchiKey:	PWJYOTPKLOICJK-UHFFFAOYSA-N
Formula:	C13H11N
SMILES:	<chem>Cc1ccc2c(c1)[nH]c1cccc12</chem>
Mol. weight [g/mol]:	181.23
CAS:	3652-91-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.78		Crippen Method
logp	3.148		Crippen Method
mcvol	145.630	ml/mol	McGowan Method
rinsol	326.94		NIST Webbook
rinsol	329.61		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3652913&Units=SI
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

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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