9H-Carbazole, 3-methoxy-

Other names:	Carbazole, 3-methoxy- 3-Methoxycarbazole
Inchi:	InChI=1S/C13H11NO/c1-15-9-6-7-13-11(8-9)10-4-2-3-5-12(10)14-13/h2-8,14H,1H3
InchiKey:	BISIQSCKDZYPLR-UHFFFAOYSA-N
Formula:	C13H11NO
SMILES:	COc1ccc2[nH]c3ccccc3c2c1
Mol. weight [g/mol]:	197.23
CAS:	18992-85-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.42		Crippen Method
logp	2.848		Crippen Method
mcvol	151.500	ml/mol	McGowan Method
tf	422.00 ± 4.00	K	NIST Webbook
tf	411.65 ± 2.00	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18992853&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
tf:	Normal melting (fusion) point

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