1H-Carbazole, 2,3,4,9-tetrahydro-

Other names: Carbazole, 1,2,3,4-tetrahydro-
1,2,3,4-Tetrahydrocarbazole
1H-Indole, 2,3-(1,4-butanediyl)-
2,3-Tetramethylene-1H-indole
2,3-Tetramethyleneindole
Carbazole, 5,6,7,8-tetrahydro-
5,6,7,8-Tetrahydrocarbazole
Tetrahydrocarbazole
NSC 17329

Inchi: InChI=1S/C12H13N/c1-3-7-11-9(5-1)10-6-2-4-8-12(10)13-11/h1,3,5,7,13H,2,4,6,8H2

InchiKey: XKLNOVWDVMWTOB-UHFFFAOYSA-N

Formula: C12H13N

SMILES: c1ccc2c3c([nH]c2c1)CCCC3

Mol. weight [g/mol]: 171.24

CAS: 942-01-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	2.565		Crippen Method
mcvol	140.140	ml/mol	McGowan Method
rinpol	306.76		NIST Webbook
rinpol	1809.00		NIST Webbook
rinpol	1800.40		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1786.60		NIST Webbook
rinpol	1800.40		NIST Webbook
rinpol	1811.80		NIST Webbook
rinpol	1786.60		NIST Webbook
rinpol	1800.40		NIST Webbook
rinpol	1811.80		NIST Webbook
rinpol	1800.40		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	306.76		NIST Webbook
tb	600.70	K	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C942018&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature