3-Methylcarbazole

Other names: 9H-Carbazole, 3-methyl-
Carbazole, 3-methyl-
3-methyl-9H-carbazole
Inchi: InChI=1S/C13H11N/c1-9-6-7-13-11(8-9)10-4-2-3-5-12(10)14-13/h2-8,14H,1H3
InchiKey: PHKYYUQQYARDIU-UHFFFAOYSA-N
Formula: C13H11N
SMILES: Cc1ccc2[nH]c3ccccc3c2c1
Mol. weight [g/mol]: 181.23
CAS: 4630-20-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.78		Crippen Method
logp	3.148		Crippen Method
mcvol	145.630	ml/mol	McGowan Method
rinpol	328.81		NIST Webbook
tf	479.00 ± 4.00	K	NIST Webbook
tf	476.15 ± 2.00	K	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4630200&Units=SI

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