9H-Carbazole, 9-butyl-

Other names: N-Butyl-carbazole
9-butyl-9H-carbazole
Inchi: InChI=1S/C16H17N/c1-2-3-12-17-15-10-6-4-8-13(15)14-9-5-7-11-16(14)17/h4-11H,2-3,1
InchiKey: SQFONLULGFXJAA-UHFFFAOYSA-N
Formula: C16H17N
SMILES: CCCCn1c2ccccc2c2ccccc21
Mol. weight [g/mol]: 223.31
CAS: 1484-08-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.18		Crippen Method
logp	4.595		Crippen Method
mcvol	187.900	ml/mol	McGowan Method
rinpol	2024.00		NIST Webbook
ripol	2834.00		NIST Webbook
ripol	2884.00		NIST Webbook
ripol	2834.00		NIST Webbook
tf	331.00 ± 4.00	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=C1484088&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
ripol:	Polar retention indices
tf:	Normal melting (fusion) point