

9H-Carbazole, 9-(1-methylethyl)-

Other names:	Carbazole, 9-isopropyl- N-Isopropylcarbazole 9-Isopropyl carbazole 9H-Carbazole, 9-isopropyl- 9-isopropyl-9H-carbazole
Inchi:	InChI=1S/C15H15N/c1-11(2)16-14-9-5-3-7-12(14)13-8-4-6-10-15(13)16/h3-11H,1-2H3
InchiKey:	LSZJZNNASZFXKN-UHFFFAOYSA-N
Formula:	C15H15N
SMILES:	CC(C)n1c2ccccc2c2ccccc21
Mol. weight [g/mol]:	209.29
CAS:	1484-09-9

Physical Properties

Property code	Value	Unit	Source
ie	7.80	eV	NIST Webbook
ie	7.40	eV	NIST Webbook
log10ws	-5.72		Crippen Method
logp	4.375		Crippen Method
mcvol	173.810	ml/mol	McGowan Method
tf	395.15 ± 1.00	K	NIST Webbook
tf	393.40 ± 4.00	K	NIST Webbook
tf	395.20 ± 0.30	K	NIST Webbook
tf	396.15 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	17.73	kJ/mol	395.20	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1484099&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
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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