

5H-BENZO[B]CARBAZOLE

Other names:	5H-Benzo[b]carbazole Benzocarbazole 2,3-Benzcarbazole 2,3-Benzocarbazole
Inchi:	InChI=1S/C16H11N/c1-2-6-12-10-16-14(9-11(12)5-1)13-7-3-4-8-15(13)17-16/h1-10,17H
InchiKey:	ROEOVWIEALGNLM-UHFFFAOYSA-N
Formula:	C16H11N
SMILES:	c1ccc2cc3c(cc2c1)[nH]c1ccccc13
Mol. weight [g/mol]:	217.27

Physical Properties

Property code	Value	Unit	Source
hf	282.06	kJ/mol	Cheméo Relay (1.0)
hvap	110.05	kJ/mol	Cheméo Relay (1.0)
ie	7.10 ± 0.10	eV	NIST Webbook
log10ws	-6.31		Cheméo Relay (1.0)
logp	3.992		Crippen Method
mcvol	168.440	ml/mol	McGowan Method
pc	3519.72	kPa	Cheméo Relay (1.0, beta)
rinpol	409.31		NIST Webbook
rinpol	410.12		NIST Webbook
rinpol	409.31		NIST Webbook
rinpol	410.12		NIST Webbook
rinpol	407.54		NIST Webbook
rinpol	409.31		NIST Webbook
rinpol	409.63		NIST Webbook
rinpol	2442.00		NIST Webbook
tb	706.89	K	Cheméo Relay (1.0)
tc	1031.05	K	Cheméo Relay (1.0)
tf	528.58	K	Cheméo Relay (1.0)
vc	0.647	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C243287&Units=SI>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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