

7H-BENZO[C]CARBAZOLE

Other names:	3,4-Benzocarbazole 7-Aza-7H-benzo[c]fluorene
Inchi:	InChI=1S/C16H11N/c1-2-6-12-11(5-1)9-10-15-16(12)13-7-3-4-8-14(13)17-15/h1-10,17H
InchiKey:	UGFOTZLGPPWNPY-UHFFFAOYSA-N
Formula:	C16H11N
SMILES:	c1ccc2c(c1)ccc1[nH]c3ccccc3c12
Mol. weight [g/mol]:	217.27

Physical Properties

Property code	Value	Unit	Source
hf	290.14	kJ/mol	Cheméo Relay (1.0)
hvap	104.38	kJ/mol	Cheméo Relay (1.0)
ie	7.15	eV	Cheméo Relay (1.0)
log10ws	-5.75		Cheméo Relay (1.0)
logp	3.992		Crippen Method
mcvol	168.440	ml/mol	McGowan Method
pc	3412.72	kPa	Cheméo Relay (1.0, beta)
tb	693.06	K	Cheméo Relay (1.0)
tc	1026.52	K	Cheméo Relay (1.0)
tf	464.45	K	Cheméo Relay (1.0)
vc	0.644	m3/kmol	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C205254&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log₁₀ws:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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