

5H-BENZO[DEF]CARBAZOLE

Other names:	Benzo[def]carbazole 4,5-Iminophenanthrene 4,5-epiminophenanthrene
Inchi:	InChI=1S/C14H9N/c1-3-9-7-8-10-4-2-6-12-14(10)13(9)11(5-1)15-12/h1-8,15H
InchiKey:	VQOUCGZKKPJLGH-UHFFFAOYSA-N
Formula:	C14H9N
SMILES:	c1cc2ccc3cccc4[nH]c(c1)c2c34
Mol. weight [g/mol]:	191.23

Physical Properties

Property code	Value	Unit	Source
hf	261.97	kJ/mol	Cheméo Relay (1.0)
hvap	91.81	kJ/mol	Cheméo Relay (1.0)
ie	7.60 ± 0.10	eV	NIST Webbook
log10ws	-5.20		Cheméo Relay (1.0)
logp	3.430		Crippen Method
mcvol	144.560	ml/mol	McGowan Method
pc	3737.51	kPa	Cheméo Relay (1.0, beta)
rinpol	363.42		NIST Webbook
rinpol	364.22		NIST Webbook
rinpol	362.82		NIST Webbook
rinpol	362.82		NIST Webbook
rinpol	361.90		NIST Webbook
rinpol	361.51		NIST Webbook
rinpol	362.82		NIST Webbook
rinpol	363.92		NIST Webbook
rinpol	363.42		NIST Webbook
tb	661.69	K	Cheméo Relay (1.0)
tc	993.70	K	Cheméo Relay (1.0)
tf	514.70	K	Cheméo Relay (1.0)
vc	0.573	m3/kmol	Cheméo Relay (1.0)

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C203656&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):
Cheméo Relay (1.0, beta):

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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