

5H-NAPHTHO[2,3-B]CARBAZOLE

Other names:	Naphtho[2,3-b]carbazole
Inchi:	InChI=1S/C20H13N/c1-2-6-14-10-16-12-20-18(11-15(16)9-13(14)5-1)17-7-3-4-8-19(17)2
InchiKey:	MEXWZXCQQQYPNG-UHFFFAOYSA-N
Formula:	C20H13N
SMILES:	c1ccc2cc3cc4c(cc3cc2c1)[nH]c1ccccc14
Mol. weight [g/mol]:	267.33

Physical Properties

Property code	Value	Unit	Source
hf	341.34	kJ/mol	Cheméo Relay (1.0)
hvap	136.74	kJ/mol	Cheméo Relay (1.0)
ie	7.00 ± 0.10	eV	NIST Webbook
log10ws	-8.06		Cheméo Relay (1.0)
logp	5.146		Crippen Method
mcvol	205.340	ml/mol	McGowan Method
pc	2781.78	kPa	Cheméo Relay (1.0, beta)
tb	782.51	K	Cheméo Relay (1.0)
tc	1137.51	K	Cheméo Relay (1.0)
tf	581.29	K	Cheméo Relay (1.0)
vc	0.789	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C248964&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
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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