5-BROMOINDOLE

Other names: 1H-indole, 5-bromo-
indole, 5-bromo-
Inchi: InChI=1S/C8H6BrN/c9-7-1-2-8-6(5-7)3-4-10-8/h1-5,10H
InchiKey: VXWVFZFZYXOBTA-UHFFFAOYSA-N
Formula: C8H6BrN
SMILES: Brc1ccc2[nH]ccc2c1
Mol. weight [g/mol]: 196.05

Physical Properties

Property code	Value	Unit	Source
hf	183.72	kJ/mol	Cheméo Relay (1.0)
hvap	77.12	kJ/mol	Cheméo Relay (1.0)
ie	7.85	eV	Cheméo Relay (1.0)
log10ws	-3.76		Cheméo Relay (1.0)
logp	2.449		Crippen Method
mcvol	112.140	ml/mol	McGowan Method
tb	571.80	K	Cheméo Relay (1.0)
tf	372.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	92.30	kJ/mol	298.15	Experimental thermochemical study of 5-bromoindole and 5-bromoindoline

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Experimental thermochemical study of 5-bromoindole and 5-bromoindoline:	https://www.doi.org/10.1016/j.jct.2008.07.016
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10075500&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point