

8-BROMO-1-NAPHTHYLAMINE

Other names:	8-bromo-1-naphthylamine
Inchi:	InChI=1S/C10H8BrN/c11-8-5-1-3-7-4-2-6-9(12)10(7)8/h1-6H,12H2
InchiKey:	FKFCNFWFJYIJU-UHFFFAOYSA-N
Formula:	C10H8BrN
SMILES:	Nc1cccc2cccc(Br)c12
Mol. weight [g/mol]:	222.09

Physical Properties

Property code	Value	Unit	Source
hf	181.99	kJ/mol	Cheméo Relay (1.0)
hfus	22.42	kJ/mol	Joback Method
hvap	77.93	kJ/mol	Cheméo Relay (1.0)
ie	7.40	eV	Cheméo Relay (1.0)
log10ws	-3.48		Cheméo Relay (1.0)
logp	3.184		Crippen Method
mcvol	136.020	ml/mol	McGowan Method
pc	4409.10	kPa	Joback Method
tb	598.41	K	Cheméo Relay (1.0)
tc	888.30	K	Cheméo Relay (1.0)
tf	353.80	K	Cheméo Relay (1.0)
vc	0.471	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.69	J/mol×K	622.51	Joback Method
cpg	304.76	J/mol×K	666.51	Joback Method
cpg	314.86	J/mol×K	710.50	Joback Method
cpg	324.11	J/mol×K	754.50	Joback Method
cpg	332.60	J/mol×K	798.49	Joback Method
cpg	340.45	J/mol×K	842.49	Joback Method
cpg	347.76	J/mol×K	886.48	Joback Method

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=C62456342&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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