

4-BROMOPYRIDINE

Other names:	Pyridine, 4-bromo-
Inchi:	InChI=1S/C5H4BrN/c6-5-1-3-7-4-2-5/h1-4H
InchiKey:	BSDGZUDFPKIYQG-UHFFFAOYSA-N
Formula:	C5H4BrN
SMILES:	Brc1ccncc1
Mol. weight [g/mol]:	158.00

Physical Properties

Property code	Value	Unit	Source
af	0.2887		Cheméo Relay (1.0)
affp	917.80	kJ/mol	NIST Webbook
basg	886.00	kJ/mol	NIST Webbook
gf	164.82	kJ/mol	Cheméo Relay (1.0, beta)
hf	167.19	kJ/mol	Cheméo Relay (1.0)
hvap	54.99	kJ/mol	Cheméo Relay (1.0)
ie	9.94 ± 0.05	eV	NIST Webbook
ie	10.00 ± 0.10	eV	NIST Webbook
log10ws	-0.52		Cheméo Relay (1.0)
logp	1.844		Crippen Method
mcvol	85.030	ml/mol	McGowan Method
pc	5245.35	kPa	Cheméo Relay (1.0, beta)
tb	446.15	K	Cheméo Relay (1.0)
tc	702.48	K	Cheméo Relay (1.0)
tf	335.90	K	Cheméo Relay (1.0)
vc	0.294	m3/kmol	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	302.20	K	0.05	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120872&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

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
gf:	Standard Gibbs free energy of formation
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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