

Pyridine, 3-bromo-

Other names:	3-Bromopyridine
Inchi:	InChI=1S/C5H4BrN/c6-5-2-1-3-7-4-5/h1-4H
InchiKey:	NYPYPOZNGOXYSU-UHFFFAOYSA-N
Formula:	C5H4BrN
SMILES:	Brc1cccnc1
Mol. weight [g/mol]:	158.00
CAS:	626-55-1

Physical Properties

Property code	Value	Unit	Source
affp	910.00	kJ/mol	NIST Webbook
basg	878.20	kJ/mol	NIST Webbook
hvap	52.10 ± 1.30	kJ/mol	NIST Webbook
ie	9.80 ± 0.10	eV	NIST Webbook
log10ws	-2.40		Crippen Method
logp	1.844		Crippen Method
mcvol	85.030	ml/mol	McGowan Method
tb	446.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	47.40	kJ/mol	368.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	342.20	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.57937e+01
Coeff. B	-4.81335e+03
Coeff. C	-1.54400e+01
Temperature range (K), min.	289.00
Temperature range (K), max.	474.63

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C626551&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

Latest version available from:

<https://www.chemeo.com/cid/62-176-8/Pyridine-3-bromo.pdf>

Generated by Cheméo on 2024-04-25 16:53:27.389658008 +0000 UTC m=+16353256.310235321.
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.