

BENZENAMINE, 4-BROMO-

Other names:	4-Bromanilinu 4-bromoaniline 4-bromophenylamine Aniline, p-bromo- aniline, 4-bromo- p-Bromophenylamine p-bromoaniline
Inchi:	InChI=1S/C6H6BrN/c7-5-1-3-6(8)4-2-5/h1-4H,8H2
InchiKey:	WDFQBORIUYODSI-UHFFFAOYSA-N
Formula:	C6H6BrN
SMILES:	Nc1ccc(Br)cc1
Mol. weight [g/mol]:	172.03

Physical Properties

Property code	Value	Unit	Source
af	0.4434		Cheméo Relay (1.0)
gf	183.19	kJ/mol	Joback Method
hf	123.12	kJ/mol	Cheméo Relay (1.0)
hfus	15.43	kJ/mol	Joback Method
hsub	79.40 ± 1.70	kJ/mol	NIST Webbook
hvap	65.64	kJ/mol	Cheméo Relay (1.0)
ie	7.70 ± 0.10	eV	NIST Webbook
log10ws	-1.83		Cheméo Relay (1.0)
logp	2.031		Crippen Method
mcvol	99.120	ml/mol	McGowan Method
pc	5470.75	kPa	Joback Method
rinpol	1248.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1248.00		NIST Webbook
tb	492.90 ± 0.60	K	NIST Webbook
tc	758.77	K	Cheméo Relay (1.0)
tf	349.55	K	Cheméo Relay (1.0)
vc	0.339	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.74	J/mol×K	507.03	Joback Method
cpg	188.96	J/mol×K	548.70	Joback Method
cpg	197.46	J/mol×K	590.37	Joback Method
cpg	205.28	J/mol×K	632.05	Joback Method
cpg	212.48	J/mol×K	673.72	Joback Method
cpg	219.10	J/mol×K	715.39	Joback Method
cpg	225.18	J/mol×K	757.06	Joback Method
hfust	16.75	kJ/mol	336.00	NIST Webbook
hfust	13.36	kJ/mol	336.00	NIST Webbook

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

New method for determination of vaporization and sublimation enthalpy of aromatic compounds at 298.15 K using solution calorimetry technique and group-additivity scheme:

<https://www.doi.org/10.1016/j.tca.2015.09.022>

McGowan Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C106401&Units=SI>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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