Acetamide, N-(4-bromophenyl)-

Other names:	1-(N-Acetylamino)-4-bromobenzene
	1-Bromo-4-acetamidobenzene
	4'-Bromoacetanilide
	4-Bromoacetanilide
	Acetamide, N-(p-bromophenyl)-
	Acetanilide, 4'-bromo-
	Acetanilide, p-bromo-
	Antisepsin
	Asepsin
	Bromoacetanilide
	Bromoanalide
	Bromoanilide
	Bromoantifebrin
	Monobromoacetanilide
	N-(4-Bromophenyl)acetamide
	N-(p-Bromophenyl)acetamide
	N-Acetyl-4-bromoaniline
	N-Acetyl-p-bromoaniline
	NSC 105442
	USAF DO-40
	p-Bromo-N-acetanilide
	p-Bromoacetanalide
	p-Bromoacetanilide
Inchi:	InChI=1S/C8H8BrNO/c1-6(11)10-8-4-2-7(9)3-5-8/h2-5H,1H3,(H,10,11)
InchiKey:	MSLICLMCQYQNPK-UHFFFAOYSA-N
Formula:	C8H8BrNO
SMILES:	CC(=O)Nc1ccc(Br)cc1
Mol. weight [g/mol]:	214.06
CAS:	103-88-8

Physical Properties

Property code	Value	Unit	Source
gf	94.05	kJ/mol	Joback Method
hf	-16.17	kJ/mol	Joback Method
hfus	22.11	kJ/mol	Joback Method
hsub	110.00 ± 4.00	kJ/mol	NIST Webbook

hvap	55.96	kJ/mol	Joback Method
ie	8.40 ± 0.20	eV	NIST Webbook
ie	8.17 ± 0.03	eV	NIST Webbook
log10ws	-3.08		Estimated Solubility Method
log10ws	-3.08		Aqueous Solubility Prediction Method
logp	2.408		Crippen Method
mcvol	128.870	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
tb	584.30	K	Joback Method
tc	822.49	K	Joback Method
tf	440.30	K	Vapor pressures and standard molar enthalpies, entropies and Gibbs energies of sublimation of three 4-substituted acetanilide derivatives
tf	440.82	K	Aqueous Solubility Prediction Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.29	J/mol×K	743.10	Joback Method
cpg	312.99	J/mol×K	782.80	Joback Method
cpg	267.43	J/mol×K	584.30	Joback Method
cpg	278.04	J/mol×K	624.00	Joback Method
cpg	287.86	J/mol×K	663.70	Joback Method
cpg	296.93	J/mol×K	703.40	Joback Method
cpg	320.08	J/mol×K	822.49	Joback Method
hfust	26.00	kJ/mol	440.30	NIST Webbook
hfust	25.80	kJ/mol	441.20	NIST Webbook
hvapt	78.00 ± 2.00	kJ/mol	480.00	NIST Webbook
hvapt	77.00 ± 1.00	kJ/mol	460.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C103888&Units=SI

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Vapor pressures and standard molar enthalpies, entropies and Gibbs energies of sublimation of three 4-substituted acetanilide derivatives:	https://www.doi.org/10.1016/j.fluid.2009.02.001
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

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
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume