Acetamide, N-(3-bromophenyl)-

Other names:	Acetanilide, 3'-bromo-
	3-Bromoacetanilide
	3'-Bromoacetanilide
	N-(3-Bromophenyl)acetic acid amide
Inchi:	InChI=1S/C8H8BrNO/c1-6(11)10-8-4-2-3-7(9)5-8/h2-5H,1H3,(H,10,11)
InchiKey:	XXHOHJTVFUJJMT-UHFFFAOYSA-N
Formula:	C8H8BrNO
SMILES:	CC(=O)Nc1cccc(Br)c1
Mol. weight [g/mol]:	214.06
CAS:	621-38-5

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
hvap	55.96	kJ/mol	Joback Method
ie	8.60 ± 0.20	eV	NIST Webbook
log10ws	-2.84		Crippen 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	381.25	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	305.29	J/mol×K	743.10	Joback Method
cpg	312.99	J/mol×K	782.80	Joback Method
cpg	320.08	J/mol×K	822.49	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C621385&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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