4'-Bromo-2'-nitroacetanilide

Other names: 4-Bromo-2-nitroacetanilide
Acetamide, N-(4-bromo-2-nitrophenyl)-
Inchi: InChI=1S/C8H7BrN2O3/c1-5(12)10-7-3-2-6(9)4-8(7)11(13)14/h2-4H,1H3,(H,10,12)
InchiKey: GUBNCRISSRANNO-UHFFFAOYSA-N
Formula: C8H7BrN2O3
SMILES: CC(=O)Nc1ccc(Br)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 259.06
CAS: 881-50-5

Physical Properties

Property code	Value	Unit	Source
gf	119.97	kJ/mol	Joback Method
hf	-38.40	kJ/mol	Joback Method
hfus	33.08	kJ/mol	Joback Method
hvap	73.21	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.316		Crippen Method
mcvol	146.290	ml/mol	McGowan Method
pc	4283.05	kPa	Joback Method
tb	741.12	K	Joback Method
tc	1000.96	K	Joback Method
tf	537.38	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.90	J/mol×K	741.12	Joback Method
cpg	354.90	J/mol×K	784.43	Joback Method
cpg	363.08	J/mol×K	827.73	Joback Method
cpg	370.51	J/mol×K	871.04	Joback Method
cpg	377.22	J/mol×K	914.35	Joback Method
cpg	383.30	J/mol×K	957.65	Joback Method
cpg	388.78	J/mol×K	1000.96	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=C881505&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
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