Acetamide, N-(4-bromo-2-nitrophenyl)-

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

Physical Properties

Property code	Value	Unit	Source
hfus	33.08	kJ/mol	Joback Method
ie	8.77	eV	Cheméo Relay (1.0)
log10ws	-3.57		Cheméo Relay (1.0)
logp	2.316		Crippen Method
mcvol	146.290	ml/mol	McGowan Method
tf	408.51	K	Cheméo Relay (1.0)

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

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C881505&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point