Benzonitrile, 4-(bromoacetyl)-

Other names:	4-Cyanophenacyl bromide
	p-Bromoacetylbenzonitrile
	Benzonitrile, 4-(2-bromoacetyl)-
	4-(2-Bromoacety)-BenZonitrile
Inchi:	InChI=1S/C9H6BrNO/c10-5-9(12)8-3-1-7(6-11)2-4-8/h1-4H,5H2
InchiKey:	LJANCPRIUMHGJE-UHFFFAOYSA-N
Formula:	C9H6BrNO
SMILES:	N#Cc1ccc(C(=O)CBr)cc1
Mol. weight [g/mol]:	224.05
CAS:	20099-89-2

Physical Properties

Property code	Value	Unit	Source
gf	146.26	kJ/mol	Joback Method
hf	74.60	kJ/mol	Joback Method
hfus	21.11	kJ/mol	Joback Method
hvap	62.23	kJ/mol	Joback Method
ie	9.90	eV	NIST Webbook
log10ws	-2.92		Crippen Method
logp	2.136		Crippen Method
mcvol	134.360	ml/mol	McGowan Method
pc	3633.35	kPa	Joback Method
tb	659.09	K	Joback Method
tc	907.81	K	Joback Method
tf	404.85	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.01	J/mol×K	659.09	Joback Method
cpg	291.76	J/mol×K	700.54	Joback Method
cpg	299.80	J/mol×K	742.00	Joback Method
cpg	307.16	J/mol×K	783.45	Joback Method

cpg	313.90	J/mol×K	824.90	Joback Method
cpg	320.07	J/mol×K	866.35	Joback Method
cpg	325.72	J/mol×K	907.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20099892&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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