4-Bromo-3'-nitroacetophenone

Other names:	4'-Bromo-3'-nitroacetophenone
	4-Bromo-3-nitroacetophenone
	Ethanone, 1-(4-bromo-3-nitrophenyl)-
	3-Nitro-4-bromoacetophenone
	Acetophenone, 4'-bromo-3'-nitro-
	1-(4-bromo-3-nitrophenyl)ethan-1-one
Inchi:	InChI=1S/C8H6BrNO3/c1-5(11)6-2-3-7(9)8(4-6)10(12)13/h2-4H,1H3
InchiKey:	YFVOFFKNHQTQQE-UHFFFAOYSA-N
Formula:	C8H6BrNO3
SMILES:	CC(=O)c1ccc(Br)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	244.04
CAS:	18640-58-9

Physical Properties

Property code	Value	Unit	Source
gf	30.58	kJ/mol	Joback Method
hf	-91.87	kJ/mol	Joback Method
hfus	27.98	kJ/mol	Joback Method
hvap	66.77	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.560		Crippen Method
mcvol	136.310	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
tb	690.95	K	Joback Method
tc	955.36	K	Joback Method
tf	484.72	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.68	J/mol×K	690.95	Joback Method
cpg	311.86	J/mol×K	735.02	Joback Method
cpg	320.21	J/mol×K	779.09	Joback Method

cpg	327.81	J/mol×K	823.16	Joback Method
cpg	334.71	J/mol×K	867.23	Joback Method
cpg	340.96	J/mol×K	911.30	Joback Method
cpg	346.60	J/mol×K	955.36	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=C18640589&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