Ethanone, 1-(4-bromophenyl)-

Other names:	1-(4-bromophenyl)ethanone
	1-acetyl-4-bromobenzene
	4'-bromoacetophenone
	4-Bromoacetophenone
	4-bromophenyl methyl ketone
	Acetophenone, 4'-bromo-
	Methyl p-bromophenyl ketone
	p-Bromoacetophenone
	p-Bromophenyl methyl ketone
Inchi:	InChI=1S/C8H7BrO/c1-6(10)7-2-4-8(9)5-3-7/h2-5H,1H3
InchiKey:	WYECURVXVYPVAT-UHFFFAOYSA-N
Formula:	C8H7BrO
SMILES:	CC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]:	199.04
CAS:	99-90-1

Physical Properties

Property code	Value	Unit	Source
gf	4.66	kJ/mol	Joback Method
hf	-69.64	kJ/mol	Joback Method
hfus	17.01	kJ/mol	Joback Method
hvap	49.52	kJ/mol	Joback Method
ie	9.50 ± 0.10	eV	NIST Webbook
ie	9.55	eV	NIST Webbook
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-3.29		Crippen Method
logp	2.652		Crippen Method
mcvol	118.890	ml/mol	McGowan Method
pc	4227.54	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1315.10		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1296.70		NIST Webbook
rinpol	1286.30		NIST Webbook
rinpol	1286.30		NIST Webbook
tb	528.20	K	NIST Webbook

tc	773.78	K	Joback Method
tf	324.00	K	NIST Webbook
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.78	J/mol×K	773.78	Joback Method
cpg	225.59	J/mol×K	534.13	Joback Method
cpg	236.06	J/mol×K	574.07	Joback Method
cpg	245.77	J/mol×K	614.01	Joback Method
cpg	254.75	J/mol×K	653.96	Joback Method
cpg	263.05	J/mol×K	693.90	Joback Method
cpg	270.71	J/mol×K	733.84	Joback Method
dvisc	0.0003200	Pa×s	534.13	Joback Method
dvisc	0.0020282	Pa×s	328.59	Joback Method
dvisc	0.0012893	Pa×s	362.85	Joback Method
dvisc	0.0008862	Pa×s	397.10	Joback Method
dvisc	0.0006465	Pa×s	431.36	Joback Method
dvisc	0.0004940	Pa×s	465.62	Joback Method
dvisc	0.0003917	Pa×s	499.87	Joback Method
hvapt	84.50	kJ/mol	298.15	Calorimetric study of bromoacetophenone isomers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	528.70	K	98.10	NIST Webbook
tbrp	528.60	K	98.10	NIST Webbook
tbrp	390.00	K	0.90	NIST Webbook

Sources

Calorimetric study of bromoacetophenone isomers: https://www.doi.org/10.1016/j.jct.2014.06.028

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=C99901&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
dvisc:	Dynamic viscosity
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume