Ethanone, 1-(3-bromophenyl)-

Other names:	1-acetyl-3-bromobenzene
	3'-bromoacetophenone
	3-bromoacetophenone
	Acetophenone, 3'-bromo-
	acetophenone, 3-bromo-
	m-bromoacetophenone
	m-bromophenyl methyl ketone
Inchi:	InChI=1S/C8H7BrO/c1-6(10)7-3-2-4-8(9)5-7/h2-5H,1H3
InchiKey:	JYAQYXOVOHJRCS-UHFFFAOYSA-N
Formula:	C8H7BrO
SMILES:	CC(=O)c1cccc(Br)c1
Mol. weight [g/mol]:	199.04
CAS:	2142-63-4

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	9.60 ± 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	1375.50		NIST Webbook
rinpol	1310.40		NIST Webbook
rinpol	1310.40		NIST Webbook
tb	534.13	K	Joback Method
tc	773.78	K	Joback Method
tf	280.50 ± 0.50	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	270.71	J/mol×K	733.84	Joback Method
cpg	263.05	J/mol×K	693.90	Joback Method
cpg	254.75	J/mol×K	653.96	Joback Method
cpg	245.77	J/mol×K	614.01	Joback Method
cpg	236.06	J/mol×K	574.07	Joback Method
cpg	225.59	J/mol×K	534.13	Joback Method
dvisc	0.0020282	Pa×s	328.59	Joback Method
dvisc	0.0003200	Pa×s	534.13	Joback Method
dvisc	0.0003917	Pa×s	499.87	Joback Method
dvisc	0.0004940	Pa×s	465.62	Joback Method
dvisc	0.0006465	Pa×s	431.36	Joback Method
dvisc	0.0008862	Pa×s	397.10	Joback Method
dvisc	0.0012893	Pa×s	362.85	Joback Method
hvapt	66.60	kJ/mol	298.15	Calorimetric study of bromoacetophenone isomers

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	404.20	K	2.10	NIST Webbook
tbrp	404.00	K	2.10	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2142634&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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

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