1-Pentanone, 1-(4-bromophenyl)-

Other names:	p-Bromophenyl butyl ketone
	1-(4-Bromophenyl)-1-pentanone
	p-Bromovalerophenone
	4'-Bromovalerophenone
	Valerophenone, 4'-bromo-
Inchi:	InChI=1S/C11H13BrO/c1-2-3-4-11(13)9-5-7-10(12)8-6-9/h5-8H,2-4H2,1H3
InchiKey:	STYJKBMRWQQJIS-UHFFFAOYSA-N
Formula:	C11H13BrO
SMILES:	CCCCC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]:	241.12
CAS:	7295-44-5

Physical Properties

Property code	Value	Unit	Source
gf	29.92	kJ/mol	Joback Method
hf	-131.56	kJ/mol	Joback Method
hfus	24.78	kJ/mol	Joback Method
hvap	56.20	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.822		Crippen Method
mcvol	161.160	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
tb	602.77	K	Joback Method
tc	828.66	K	Joback Method
tf	362.40	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.69	J/mol×K	602.77	Joback Method
cpg	374.02	J/mol×K	640.42	Joback Method
cpg	386.45	J/mol×K	678.07	Joback Method
cpg	398.05	J/mol×K	715.71	Joback Method

cpg	408.86	J/mol×K	753.36	Joback Method
cpg	418.92	J/mol×K	791.01	Joback Method
cpg	428.28	J/mol×K	828.66	Joback Method
dvisc	0.0018845	Pa×s	362.40	Joback Method
dvisc	0.0011309	Pa×s	402.46	Joback Method
dvisc	0.0007443	Pa×s	442.52	Joback Method
dvisc	0.0005252	Pa×s	482.59	Joback Method
dvisc	0.0003909	Pa×s	522.65	Joback Method
dvisc	0.0003034	Pa×s	562.71	Joback Method
dvisc	0.0002436	Pa×s	602.77	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	441.70	K	2.70	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7295445&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
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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume