

1-Propanone, 1-(4-bromophenyl)-

Other names:	Propiophenone, 4'-bromo- p-Bromopropiophenone 4'-Bromopropiophenone 4-Bromopropiophenone
Inchi:	InChI=1S/C9H9BrO/c1-2-9(11)7-3-5-8(10)6-4-7/h3-6H,2H2,1H3
InchiKey:	UOMOSYFPKGQIKI-UHFFFAOYSA-N
Formula:	C9H9BrO
SMILES:	CCC(=O)c1ccc(Br)cc1
Mol. weight [g/mol]:	213.07
CAS:	10342-83-3

Physical Properties

Property code	Value	Unit	Source
gf	13.08	kJ/mol	Joback Method
hf	-90.28	kJ/mol	Joback Method
hfus	19.60	kJ/mol	Joback Method
hvap	51.75	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.042		Crippen Method
mcvol	132.980	ml/mol	McGowan Method
pc	3745.38	kPa	Joback Method
tb	557.01	K	Joback Method
tc	791.91	K	Joback Method
tf	339.86	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.87	J/molxK	557.01	Joback Method
cpg	318.99	J/molxK	752.76	Joback Method
cpg	310.41	J/molxK	713.61	Joback Method
cpg	301.16	J/molxK	674.46	Joback Method
cpg	291.18	J/molxK	635.31	Joback Method

cpg	280.43	J/molxK	596.16	Joback Method
cpg	326.92	J/molxK	791.91	Joback Method
dvisc	0.0002945	Paxs	557.01	Joback Method
dvisc	0.0003627	Paxs	520.82	Joback Method
dvisc	0.0004609	Paxs	484.63	Joback Method
dvisc	0.0006088	Paxs	448.44	Joback Method
dvisc	0.0008444	Paxs	412.24	Joback Method
dvisc	0.0012473	Paxs	376.05	Joback Method
dvisc	0.0020020	Paxs	339.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	412.20	K	1.90	NIST Webbook
tbrp	442.20	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10342833&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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