Benzoyl chloride, 4-bromo-

Other names:	4-Bromobenzoyl chloride
	p-Bromobenzoyl chloride
	p-Bromobenzoyl chloride, p-bromo-
	Benzoyl chloride, p-bromo-
Inchi:	InChI=1S/C7H4BrClO/c8-6-3-1-5(2-4-6)7(9)10/h1-4H
InchiKey:	DENKGPBHLYFNGK-UHFFFAOYSA-N
Formula:	C7H4BrClO
SMILES:	O=C(Cl)c1ccc(Br)cc1
Mol. weight [g/mol]:	219.46
CAS:	586-75-4

Physical Properties

Property code	Value	Unit	Source
gf	-15.69	kJ/mol	Joback Method
hf	-64.74	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.828		Crippen Method
mcvol	117.040	ml/mol	McGowan Method
pc	4571.55	kPa	Joback Method
tb	519.20	K	NIST Webbook
tc	797.84	K	Joback Method
tf	310.70 ± 1.00	K	NIST Webbook
tf	315.00 ± 4.00	K	NIST Webbook
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.65	J/mol×K	548.68	Joback Method
cpg	240.03	J/mol×K	756.31	Joback Method
cpg	234.19	J/mol×K	714.78	Joback Method
cpg	227.77	J/mol×K	673.26	Joback Method

cpg	220.74	J/mol×K	631.73	Joback Method
cpg	213.05	J/mol×K	590.21	Joback Method
cpg	245.35	J/mol×K	797.84	Joback Method
dvisc	0.0003415	Pa×s	548.68	Joback Method
dvisc	0.0004156	Pa×s	515.11	Joback Method
dvisc	0.0005199	Pa×s	481.53	Joback Method
dvisc	0.0006725	Pa×s	447.96	Joback Method
dvisc	0.0009070	Pa×s	414.39	Joback Method
dvisc	0.0012896	Pa×s	380.81	Joback Method
dvisc	0.0019626	Pa×s	347.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	447.20	K	13.60	NIST Webbook

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=C586754&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
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