

O-bromobenzoyl chloride

Other names:	2-bromobenzoyl chloride
Inchi:	InChI=1S/C7H4BrClO/c8-6-4-2-1-3-5(6)7(9)10/h1-4H
InchiKey:	NZCKTGCKFJDGFD-UHFFFAOYSA-N
Formula:	C7H4BrClO
SMILES:	O=C(Cl)c1cccc1Br
Mol. weight [g/mol]:	219.46
CAS:	7154-66-7

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	518.20	K	NIST Webbook
tb	518.00	K	NIST Webbook
tc	797.84	K	Joback Method
tf	284.00	K	NIST Webbook
vc	0.436	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.65	J/mol×K	548.68	Joback Method
cpg	213.05	J/mol×K	590.21	Joback Method
cpg	220.74	J/mol×K	631.73	Joback Method
cpg	227.77	J/mol×K	673.26	Joback Method
cpg	234.19	J/mol×K	714.78	Joback Method
cpg	240.03	J/mol×K	756.31	Joback Method
cpg	245.35	J/mol×K	797.84	Joback Method

dvisc	0.0019626	Paxs	347.24	Joback Method
dvisc	0.0012896	Paxs	380.81	Joback Method
dvisc	0.0009070	Paxs	414.39	Joback Method
dvisc	0.0006725	Paxs	447.96	Joback Method
dvisc	0.0005199	Paxs	481.53	Joback Method
dvisc	0.0004156	Paxs	515.11	Joback Method
dvisc	0.0003415	Paxs	548.68	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.00	K	2.70	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7154667&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

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
mccvol:	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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