

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:	DENKGPBHLFYNGK-UHFFFAOYSA-N
Formula:	C7H4BrClO
SMILES:	O=C(Cl)c1ccc(Br)cc1
Mol. weight [g/mol]:	219.47

Physical Properties

Property code	Value	Unit	Source
hf	-92.75	kJ/mol	Cheméo Relay (1.0)
hfus	18.62	kJ/mol	Joback Method
hvap	68.49	kJ/mol	Cheméo Relay (1.0)
ie	9.57	eV	Cheméo Relay (1.0)
log10ws	-3.48		Cheméo Relay (1.0)
logp	2.828		Crippen Method
mcvol	117.040	ml/mol	McGowan Method
tb	509.93	K	Cheméo Relay (1.0)
tf	330.44	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	204.65	J/mol×K	548.68	Joback Method
cpg	245.35	J/mol×K	797.84	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
dvisc	0.0006725	Pa×s	447.96	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	0.0019626	Pa×s	347.24	Joback Method
dvisc	0.0009070	Pa×s	414.39	Joback Method
dvisc	0.0012896	Pa×s	380.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C586754&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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