

2-Iodobenzoyl chloride

Other names:	o-Iodobenzoyl chloride Benzoyl chloride, 2-iodo-
Inchi:	InChI=1S/C7H4ClIO/c8-7(10)5-3-1-2-4-6(5)9/h1-4H
InchiKey:	MVIVDSWUOGNODP-UHFFFAOYSA-N
Formula:	C7H4ClIO
SMILES:	O=C(Cl)c1ccccc1I
Mol. weight [g/mol]:	266.46
CAS:	609-67-6

Physical Properties

Property code	Value	Unit	Source
gf	28.11	kJ/mol	Joback Method
hf	-14.20	kJ/mol	Joback Method
hfus	17.74	kJ/mol	Joback Method
hvap	54.62	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.670		Crippen Method
mcvol	125.360	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
tb	575.66	K	Joback Method
tc	842.84	K	Joback Method
tf	345.50	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.94	J/mol×K	575.66	Joback Method
cpg	220.21	J/mol×K	620.19	Joback Method
cpg	227.70	J/mol×K	664.72	Joback Method
cpg	234.47	J/mol×K	709.25	Joback Method
cpg	240.60	J/mol×K	753.78	Joback Method
cpg	246.13	J/mol×K	798.31	Joback Method
cpg	251.12	J/mol×K	842.84	Joback Method

dvisc	0.0024862	Pa×s	345.50	Joback Method
dvisc	0.0015097	Pa×s	383.86	Joback Method
dvisc	0.0010037	Pa×s	422.22	Joback Method
dvisc	0.0007143	Pa×s	460.58	Joback Method
dvisc	0.0005356	Pa×s	498.94	Joback Method
dvisc	0.0004185	Pa×s	537.30	Joback Method
dvisc	0.0003379	Pa×s	575.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.70	K	0.10	NIST Webbook
tbrp	432.20	K	3.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C609676&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

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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