

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0024862	Paxs	345.50	Joback Method
dvisc	0.0015097	Paxs	383.86	Joback Method
dvisc	0.0010037	Paxs	422.22	Joback Method
dvisc	0.0007143	Paxs	460.58	Joback Method
dvisc	0.0005356	Paxs	498.94	Joback Method
dvisc	0.0004185	Paxs	537.30	Joback Method
dvisc	0.0003379	Paxs	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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C609676&Units=SI

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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