4-Chloro-2-iodobenzoic acid

Inchi: InChI=1S/C7H4ClIO2/c8-4-1-2-5(7(10)11)6(9)3-4/h1-3H,(H,10,11)
InchiKey: LRRDANNSUCQNDU-UHFFFAOYSA-N
Formula: C7H4ClIO2
SMILES: O=C(O)c1ccc(Cl)cc1I
Mol. weight [g/mol]: 282.46
CAS: 13421-13-1

Physical Properties

Property code	Value	Unit	Source
gf	-118.34	kJ/mol	Joback Method
hf	-177.90	kJ/mol	Joback Method
hfus	21.44	kJ/mol	Joback Method
hvap	71.96	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	2.643		Crippen Method
mcvol	131.230	ml/mol	McGowan Method
pc	4486.22	kPa	Joback Method
tb	672.82	K	Joback Method
tc	915.10	K	Joback Method
tf	418.84	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.40	J/mol×K	672.82	Joback Method
cpg	249.60	J/mol×K	713.20	Joback Method
cpg	255.29	J/mol×K	753.58	Joback Method
cpg	260.49	J/mol×K	793.96	Joback Method
cpg	265.26	J/mol×K	834.34	Joback Method
cpg	269.62	J/mol×K	874.72	Joback Method
cpg	273.61	J/mol×K	915.10	Joback Method
dvisc	0.0018874	Pa×s	418.84	Joback Method
dvisc	0.0008973	Pa×s	461.17	Joback Method

dvisc	0.0004834	Pa×s	503.50	Joback Method
dvisc	0.0002866	Pa×s	545.83	Joback Method
dvisc	0.0001833	Pa×s	588.16	Joback Method
dvisc	0.0001244	Pa×s	630.49	Joback Method
dvisc	0.0000887	Pa×s	672.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13421131&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume