

2-Chloro-5-iodobenzoic acid

Other names:	Benzoic acid, 2-chloro-5-iodo-
Inchi:	InChI=1S/C7H4ClIO2/c8-6-2-1-4(9)3-5(6)7(10)11/h1-3H,(H,10,11)
InchiKey:	GEBYSTBEDVQOTK-UHFFFAOYSA-N
Formula:	C7H4ClIO2
SMILES:	O=C(O)c1cc(I)ccc1Cl
Mol. weight [g/mol]:	282.46
CAS:	19094-56-5

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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.40	J/mol×K	672.82	Joback Method
cpg	269.62	J/mol×K	874.72	Joback Method
cpg	265.26	J/mol×K	834.34	Joback Method
cpg	260.49	J/mol×K	793.96	Joback Method
cpg	255.29	J/mol×K	753.58	Joback Method
cpg	249.60	J/mol×K	713.20	Joback Method
cpg	273.61	J/mol×K	915.10	Joback Method
dvisc	0.0000887	Paxs	672.82	Joback Method

dvisc	0.0001244	Paxs	630.49	Joback Method
dvisc	0.0001833	Paxs	588.16	Joback Method
dvisc	0.0002866	Paxs	545.83	Joback Method
dvisc	0.0004834	Paxs	503.50	Joback Method
dvisc	0.0008973	Paxs	461.17	Joback Method
dvisc	0.0018874	Paxs	418.84	Joback Method

Sources

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=C19094565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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