Benzoic acid, 3-iodo-

Other names: 3-Iodobenzoic acid
Benzoic acid, m-iodo-
m-Iodobenzoic acid
Inchi: InChI=1S/C7H5IO2/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)
InchiKey: KVBWBCRPWVKFQT-UHFFFAOYSA-N
Formula: C7H5IO2
SMILES: O=C(O)c1cccc(I)c1
Mol. weight [g/mol]: 248.02
CAS: 618-51-9

Physical Properties

Property code	Value	Unit	Source
chs	-3152.00 ± 3.00	kJ/mol	NIST Webbook
chs	-3153.80 ± 2.20	kJ/mol	NIST Webbook
gf	-96.78	kJ/mol	Joback Method
hf	-219.00 ± 2.20	kJ/mol	NIST Webbook
hfs	-315.40 ± 2.20	kJ/mol	NIST Webbook
hfus	17.63	kJ/mol	Joback Method
hsub	96.40 ± 0.30	kJ/mol	NIST Webbook
hsub	111.10 ± 1.90	kJ/mol	NIST Webbook
hvap	66.91	kJ/mol	Joback Method
log10ws	-3.27		Aqueous Solubility Prediction Method
logp	1.989		Crippen Method
mcvol	118.990	ml/mol	McGowan Method
pc	4815.84	kPa	Joback Method
tb	630.41	K	Joback Method
tc	868.95	K	Joback Method
tf	458.90	K	Thermochemistry of halogenobenzoic acids as an access to PC-SAFT solubility modeling
tf	460.58	K	Aqueous Solubility Prediction Method
tt	460.30 ± 0.01	K	NIST Webbook
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.84	J/mol×K	868.95	Joback Method
cpg	227.76	J/mol×K	630.41	Joback Method
cpg	234.94	J/mol×K	670.17	Joback Method
cpg	241.53	J/mol×K	709.92	Joback Method
cpg	247.57	J/mol×K	749.68	Joback Method
cpg	253.10	J/mol×K	789.44	Joback Method
cpg	258.18	J/mol×K	829.20	Joback Method
dvisc	0.0001104	Pa×s	630.41	Joback Method
dvisc	0.0036678	Pa×s	376.40	Joback Method
dvisc	0.0015227	Pa×s	418.74	Joback Method
dvisc	0.0007429	Pa×s	461.07	Joback Method
dvisc	0.0004089	Pa×s	503.41	Joback Method
dvisc	0.0002470	Pa×s	545.74	Joback Method
dvisc	0.0001604	Pa×s	588.08	Joback Method
hfust	28.70	kJ/mol	460.40	NIST Webbook
hsubt	109.60 ± 0.50	kJ/mol	355.00	NIST Webbook

Sources

Thermochemistry of halogenobenzoic acids as an access to PC-SAFT solubility modeling: https://www.doi.org/10.1016/j.fluid.2015.10.001

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C618519&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
tt:	Triple Point Temperature
vc:	Critical Volume