Benzoic acid, 4-iodo-

Other names:	4-Jodbenzoesaeure
	4-iodobenzoic acid
	Benzoic acid, p-iodo-
	p-Iodobenzenecarboxylic acid
	p-iodobenzoic acid
Inchi:	InChI=1S/C7H5IO2/c8-6-3-1-5(2-4-6)7(9)10/h1-4H,(H,9,10)
InchiKey:	GHICCUXQJBDNRN-UHFFFAOYSA-N
Formula:	C7H5IO2
SMILES:	O=C(O)c1ccc(I)cc1
Mol. weight [g/mol]:	248.02
CAS:	619-58-9

Physical Properties

Property code	Value	Unit	Source
chs	-3154.20 ± 1.30	kJ/mol	NIST Webbook
chs	-3153.00 ± 3.00	kJ/mol	NIST Webbook
gf	-96.78	kJ/mol	Joback Method
hf	-215.60 ± 1.30	kJ/mol	NIST Webbook
hf	-228.00 ± 5.90	kJ/mol	NIST Webbook
hfl	-316.00 ± 4.20	kJ/mol	NIST Webbook
hfs	-314.90 ± 1.30	kJ/mol	NIST Webbook
hfus	17.63	kJ/mol	Joback Method
hsub	112.90 ± 2.50	kJ/mol	NIST Webbook
hsub	99.30 ± 0.40	kJ/mol	NIST Webbook
hvap	87.90 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.68		Crippen 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	543.90	K	Thermochemistry of halogenobenzoic acids as an access to PC-SAFT solubility modeling
tt	543.70 ± 0.03	K	NIST Webbook
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.57	J/mol×K	749.68	Joback Method
cpg	262.84	J/mol×K	868.95	Joback Method
cpg	258.18	J/mol×K	829.20	Joback Method
cpg	253.10	J/mol×K	789.44	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
dvisc	0.0001104	Pa×s	630.41	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
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
hfust	35.24	kJ/mol	543.80	NIST Webbook
hfust	35.24	kJ/mol	543.80	NIST Webbook
hfust	33.94	kJ/mol	544.74	NIST Webbook
hsubt	111.00 ± 0.40	kJ/mol	371.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C619589&Units=SI

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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

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
hfl:	Liquid phase 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