Propanoic acid, 3-iodo-

Other names:	3-Iodopropanoic acid
	3-Iodopropionic acid
	Beta-iodopropionic acid
	Propionic acid, 3-iodo-
	«beta»-Iodopropionic acid
	Â«betaÂ»-Iodopropionic acid
Inchi:	InChI=1S/C3H5IO2/c4-2-1-3(5)6/h1-2H2,(H,5,6)
InchiKey:	KMRNTNDWADEIIX-UHFFFAOYSA-N
Formula:	C3H5IO2
SMILES:	O=C(O)CCI
Mol. weight [g/mol]:	199.98
CAS:	141-76-4

Physical Properties

Property code	Value	Unit	Source
chs	-1435.10 ± 5.00	kJ/mol	NIST Webbook
gf	-233.24	kJ/mol	Joback Method
hf	-293.19	kJ/mol	Joback Method
hfs	-460.00 ± 5.00	kJ/mol	NIST Webbook
hfus	13.62	kJ/mol	Joback Method
hvap	55.07	kJ/mol	Joback Method
log10ws	-0.43		Aqueous Solubility Prediction Method
logp	0.896		Crippen Method
mcvol	86.390	ml/mol	McGowan Method
pc	5304.68	kPa	Joback Method
tb	507.23	K	Joback Method
tc	713.74	K	Joback Method
tf	354.90	K	Aqueous Solubility Prediction Method
vc	0.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	142.50	J/mol×K	507.23	Joback Method
cpg	147.45	J/mol×K	541.65	Joback Method
cpg	152.09	J/mol×K	576.07	Joback Method
cpg	156.46	J/mol×K	610.49	Joback Method
cpg	160.55	J/mol×K	644.91	Joback Method
cpg	164.39	J/mol×K	679.33	Joback Method
cpg	168.00	J/mol×K	713.74	Joback Method
dvisc	0.0189507	Pa×s	292.38	Joback Method
dvisc	0.0063876	Pa×s	328.19	Joback Method
dvisc	0.0026667	Pa×s	364.00	Joback Method
dvisc	0.0013019	Pa×s	399.81	Joback Method
dvisc	0.0007151	Pa×s	435.61	Joback Method
dvisc	0.0004302	Pa×s	471.42	Joback Method
dvisc	0.0002781	Pa×s	507.23	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C141764&Units=SI

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

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

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

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

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