4-Iodophenylacetic acid

Other names: Benzeneacetic acid, 4-iodo-
Inchi: InChI=1S/C8H7IO2/c9-7-3-1-6(2-4-7)5-8(10)11/h1-4H,5H2,(H,10,11)
InchiKey: FJSHTWVDFAUNCO-UHFFFAOYSA-N
Formula: C8H7IO2
SMILES: O=C(O)Cc1ccc(I)cc1
Mol. weight [g/mol]: 262.04
CAS: 1798-06-7

Physical Properties

Property code	Value	Unit	Source
gf	-88.36	kJ/mol	Joback Method
hf	-171.33	kJ/mol	Joback Method
hfus	20.22	kJ/mol	Joback Method
hvap	69.14	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.918		Crippen Method
mcvol	133.080	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	653.29	K	Joback Method
tc	886.96	K	Joback Method
tf	387.67	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.22	J/mol×K	653.29	Joback Method
cpg	308.22	J/mol×K	848.02	Joback Method
cpg	302.31	J/mol×K	809.07	Joback Method
cpg	295.90	J/mol×K	770.13	Joback Method
cpg	288.94	J/mol×K	731.18	Joback Method
cpg	281.40	J/mol×K	692.24	Joback Method
cpg	313.68	J/mol×K	886.96	Joback Method
dvisc	0.0000920	Pa×s	653.29	Joback Method

dvisc	0.0001338	Pa×s	609.02	Joback Method
dvisc	0.0002065	Pa×s	564.75	Joback Method
dvisc	0.0003428	Pa×s	520.48	Joback Method
dvisc	0.0006255	Pa×s	476.21	Joback Method
dvisc	0.0012911	Pa×s	431.94	Joback Method
dvisc	0.0031447	Pa×s	387.67	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1798067&Units=SI

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