Phenol, 3-iodo-

Other names:	Phenol, m-iodo-
	m-Hydroxyiodobenzene
	m-Iodophenol
	3-Iodophenol
	3-Jodphenol
Inchi:	InChI=1S/C6H5IO/c7-5-2-1-3-6(8)4-5/h1-4,8H
InchiKey:	FXTKWBZFNQHAAO-UHFFFAOYSA-N
Formula:	C6H5IO
SMILES:	Oc1cccc(I)c1
Mol. weight [g/mol]:	220.01
CAS:	626-02-8

Physical Properties

Property code	Value	Unit	Source
chs	-2981.10 ± 4.20	kJ/mol	NIST Webbook
gf	15.55	kJ/mol	Joback Method
hf	-31.08	kJ/mol	Joback Method
hfus	15.53	kJ/mol	Joback Method
hvap	53.61	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	1.997		Crippen Method
mcvol	103.330	ml/mol	McGowan Method
pc	5602.57	kPa	Joback Method
rinpol	1369.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1369.00		NIST Webbook
rinpol	1369.00		NIST Webbook
tb	537.12	K	Joback Method
tc	808.34	K	Joback Method
tf	353.58	K	Joback Method
vc	0.318	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.45	J/mol×K	537.12	Joback Method
cpg	190.59	J/mol×K	582.32	Joback Method
cpg	197.83	J/mol×K	627.53	Joback Method
cpg	204.31	J/mol×K	672.73	Joback Method
cpg	210.19	J/mol×K	717.93	Joback Method
cpg	215.59	J/mol×K	763.14	Joback Method
cpg	220.68	J/mol×K	808.34	Joback Method
dvisc	0.0035242	Pa×s	353.58	Joback Method
dvisc	0.0015054	Pa×s	384.17	Joback Method
dvisc	0.0007290	Pa×s	414.76	Joback Method
dvisc	0.0003900	Pa×s	445.35	Joback Method
dvisc	0.0002261	Pa×s	475.94	Joback Method
dvisc	0.0001400	Pa×s	506.53	Joback Method
dvisc	0.0000916	Pa×s	537.12	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=C626028&Units=SI

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
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
rinpol: Non-polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume