Phenol, 2-iodo-

Other names:	Phenol, o-iodo-
	o-Iodophenol
	2-Iodophenol
	o-Jodfenol
	2-Jodfenol
Inchi:	InChI=1S/C6H5IO/c7-5-3-1-2-4-6(5)8/h1-4,8H
InchiKey:	KQDJTBPASNJQFQ-UHFFFAOYSA-N
Formula:	C6H5IO
SMILES:	Oc1ccccc1I
Mol. weight [g/mol]:	220.01
CAS:	533-58-4

Physical Properties

Property code	Value	Unit	Source
chs	-2979.80 ± 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	1182.00		NIST Webbook
rinpol	1163.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1163.00		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	215.59	J/mol×K	763.14	Joback Method
cpg	210.19	J/mol×K	717.93	Joback Method
cpg	204.31	J/mol×K	672.73	Joback Method
cpg	197.83	J/mol×K	627.53	Joback Method
cpg	190.59	J/mol×K	582.32	Joback Method
cpg	220.68	J/mol×K	808.34	Joback Method
dvisc	0.0000916	Pa×s	537.12	Joback Method
dvisc	0.0001400	Pa×s	506.53	Joback Method
dvisc	0.0002261	Pa×s	475.94	Joback Method
dvisc	0.0003900	Pa×s	445.35	Joback Method
dvisc	0.0007290	Pa×s	414.76	Joback Method
dvisc	0.0015054	Pa×s	384.17	Joback Method
dvisc	0.0035242	Pa×s	353.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	459.70	K	21.30	NIST Webbook

Sources

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=C533584&Units=SI

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

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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume