M-IODOPHENOL

Other names: 3-Iodophenol
3-Jodphenol
Phenol, m-iodo-
m-Hydroxyiodobenzene
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

Physical Properties

Property code	Value	Unit	Source
af	0.4559		Cheméo Relay (1.0)
chs	-2981.10 ± 4.20	kJ/mol	NIST Webbook
gf	15.55	kJ/mol	Joback Method
hf	0.63	kJ/mol	Cheméo Relay (1.0)
hfus	15.53	kJ/mol	Joback Method
hvap	73.46	kJ/mol	Cheméo Relay (1.0)
ie	8.40	eV	Cheméo Relay (1.0)
log10ws	-1.76		Cheméo Relay (1.0)
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	536.00	K	Cheméo Relay (1.0)
tc	825.16	K	Cheméo Relay (1.0)
tf	334.22	K	Cheméo Relay (1.0)
vc	0.331	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.59	J/mol×K	763.14	Joback Method
cpg	220.68	J/mol×K	808.34	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	182.45	J/mol×K	537.12	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
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
hvapt	88.40	kJ/mol	298.15	Experimental and Computational Thermochemical Study of the Three Monoiodophenol Isomers

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Experimental and Computational Thermochemical Study of the Three Monoiodophenol Isomers: https://www.doi.org/10.1021/je200833s

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626028&Units=SI

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

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

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

Legend

af: Acentric Factor

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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