Phenol, 2,4,6-triiodo-

Other names: 2,4,6-Triiodophenol
2,4,6-Trijodfenol
Inchi: InChI=1S/C6H3I3O/c7-3-1-4(8)6(10)5(9)2-3/h1-2,10H
InchiKey: VAPDZNUFNKUROY-UHFFFAOYSA-N
Formula: C6H3I3O
SMILES: Oc1c(I)cc(I)cc1I
Mol. weight [g/mol]: 471.80
CAS: 609-23-4

Physical Properties

Property code	Value	Unit	Source
gf	112.53	kJ/mol	Joback Method
hf	99.72	kJ/mol	Joback Method
hfus	23.56	kJ/mol	Joback Method
hvap	73.68	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.206		Crippen Method
mcvol	154.970	ml/mol	McGowan Method
pc	5029.93	kPa	Joback Method
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
tb	733.36	K	Joback Method
tc	1072.25	K	Joback Method
tf	494.74	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.38	J/mol×K	733.36	Joback Method
cpg	235.09	J/mol×K	789.84	Joback Method
cpg	239.70	J/mol×K	846.32	Joback Method
cpg	244.51	J/mol×K	902.80	Joback Method

cpg	249.85	J/mol×K	959.29	Joback Method
cpg	256.02	J/mol×K	1015.77	Joback Method
cpg	263.34	J/mol×K	1072.25	Joback Method
dvisc	0.0003621	Pa×s	494.74	Joback Method
dvisc	0.0001873	Pa×s	534.51	Joback Method
dvisc	0.0001061	Pa×s	574.28	Joback Method
dvisc	0.0000647	Pa×s	614.05	Joback Method
dvisc	0.0000419	Pa×s	653.82	Joback Method
dvisc	0.0000285	Pa×s	693.59	Joback Method
dvisc	0.0000202	Pa×s	733.36	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=C609234&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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