Phenol, 2,3,5-trichloro-

Other names: 2,3,5-Trichlorophenol
Inchi: InChI=1S/C6H3Cl3O/c7-3-1-4(8)6(9)5(10)2-3/h1-2,10H
InchiKey: WWGQHTJIFOQAOC-UHFFFAOYSA-N
Formula: C6H3Cl3O
SMILES: Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 197.45
CAS: 933-78-8

Physical Properties

Property code	Value	Unit	Source
gf	-97.62	kJ/mol	Joback Method
hf	-178.11	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	58.72	kJ/mol	Joback Method
log10ws	-2.67		Estimated Solubility Method
log10ws	-2.67		Aqueous Solubility Prediction Method
logp	3.352		Crippen Method
mcvol	114.230	ml/mol	McGowan Method
pc	4723.61	kPa	Joback Method
rinpol	1362.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1317.00		NIST Webbook
rinpol	1327.00		NIST Webbook
rinpol	1347.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1313.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1334.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1367.00		NIST Webbook
rinpol	1351.30		NIST Webbook
rinpol	1323.00		NIST Webbook
ripol	2389.00		NIST Webbook
ripol	2368.00		NIST Webbook
ripol	2403.00		NIST Webbook

ripol	2403.00		NIST Webbook
ripol	2410.00		NIST Webbook
ripol	2403.00		NIST Webbook
ripol	2399.00		NIST Webbook
tb	521.70	K	NIST Webbook
tc	818.35	K	Joback Method
tf	410.32	K	Joback Method
vc	0.377	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.55	J/mol×K	566.23	Joback Method
cpg	229.51	J/mol×K	776.33	Joback Method
cpg	225.09	J/mol×K	734.31	Joback Method
cpg	220.38	J/mol×K	692.29	Joback Method
cpg	215.28	J/mol×K	650.27	Joback Method
cpg	209.69	J/mol×K	608.25	Joback Method
cpg	233.71	J/mol×K	818.35	Joback Method
dvisc	0.0000638	Pa×s	566.23	Joback Method
dvisc	0.0000884	Pa×s	540.25	Joback Method
dvisc	0.0001265	Pa×s	514.26	Joback Method
dvisc	0.0001881	Pa×s	488.28	Joback Method
dvisc	0.0002925	Pa×s	462.29	Joback Method
dvisc	0.0004792	Pa×s	436.31	Joback Method
dvisc	0.0008360	Pa×s	410.32	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C933788&Units=SI

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

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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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

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