TETRACHLOROPYROCATECHOL

Other names:	Pyrocatechol, tetrachloro-
	Tetrachloro-1,2-benzenediol
	Tetrachlorocatechol
	Tetrachloropyrocatechol
	3,4,5,6-Tetrachloro-1,2-benzenediol
	Tetrachlorpyrokatechin
	Tetrachlorpyrokatechol
Inchi:	InChI=1S/C6H2Cl4O2/c7-1-2(8)4(10)6(12)5(11)3(1)9/h11-12H
InchiKey:	RRBMVWQICIXSEO-UHFFFAOYSA-N
Formula:	C6H2Cl4O2
SMILES:	Oc1c(O)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	247.89

Physical Properties

Property code	Value	Unit	Source
af	0.7051		Cheméo Relay (1.0)
hf	-330.73	kJ/mol	Cheméo Relay (1.0)
hfus	32.52	kJ/mol	Joback Method
hvap	99.23	kJ/mol	Cheméo Relay (1.0)
ie	8.66	eV	Cheméo Relay (1.0)
log10ws	-3.63		Cheméo Relay (1.0)
logp	3.711		Crippen Method
mcvol	132.340	ml/mol	McGowan Method
pc	5422.51	kPa	Joback Method
tb	555.67	K	Cheméo Relay (1.0)
tc	895.74	K	Cheméo Relay (1.0)
tf	456.42	K	Cheméo Relay (1.0)
vc	0.473	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.27	J/mol×K	689.26	Joback Method
cpg	273.16	J/mol×K	953.67	Joback Method

cpg	268.15	J/mol×K	909.61	Joback Method
cpg	263.62	J/mol×K	865.54	Joback Method
cpg	259.44	J/mol×K	821.47	Joback Method
cpg	255.42	J/mol×K	777.40	Joback Method
cpg	251.42	J/mol×K	733.33	Joback Method
dvisc	0.0000076	Pa×s	626.87	Joback Method
dvisc	0.0000030	Pa×s	689.26	Joback Method
dvisc	0.0000040	Pa×s	668.46	Joback Method
dvisc	0.0000055	Pa×s	647.67	Joback Method
dvisc	0.0000238	Pa×s	564.48	Joback Method
dvisc	0.0000108	Pa×s	606.07	Joback Method
dvisc	0.0000158	Pa×s	585.28	Joback Method
hvapt	77.90	kJ/mol	308.00	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1198556&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
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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

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