1,2-Benzenediol, 4,5-dichloro-

Other names:	Pyrocatechol, 4,5-dichloro-
	4,5-Dichlorocatechol
	4,5-Dichloropyrocatechol
	4,5-Dichloro-benzene-1,2-diol
	4,5-Dichloro-1,2-benzenediol
Inchi:	InChI=1S/C6H4Cl2O2/c7-3-1-5(9)6(10)2-4(3)8/h1-2,9-10H
InchiKey:	ACCHWUWBKYGKNM-UHFFFAOYSA-N
Formula:	C6H4Cl2O2
SMILES:	Oc1cc(Cl)c(Cl)cc1O
Mol. weight [g/mol]:	179.00
CAS:	3428-24-8

Physical Properties

Property code	Value	Unit	Source
gf	-230.68	kJ/mol	Joback Method
hf	-328.21	kJ/mol	Joback Method
hfus	24.91	kJ/mol	Joback Method
hvap	66.69	kJ/mol	Joback Method
log10ws	-1.94		Crippen Method
logp	2.405		Crippen Method
mcvol	107.860	ml/mol	McGowan Method
pc	6359.24	kPa	Joback Method
tb	604.44	K	Joback Method
tc	861.92	K	Joback Method
tf	479.60	K	Joback Method
vc	0.293	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.80	J/mol×K	861.92	Joback Method
cpg	220.56	J/mol×K	604.44	Joback Method
cpg	226.43	J/mol×K	647.35	Joback Method
cpg	231.76	J/mol×K	690.27	Joback Method

cpg	236.70	J/mol×K	733.18	Joback Method
cpg	241.40	J/mol×K	776.09	Joback Method
cpg	246.05	J/mol×K	819.00	Joback Method
dvisc	0.0000081	Pa×s	604.44	Joback Method
dvisc	0.0001179	Pa×s	479.60	Joback Method
dvisc	0.0000687	Pa×s	500.41	Joback Method
dvisc	0.0000418	Pa×s	521.21	Joback Method
dvisc	0.0000264	Pa×s	542.02	Joback Method
dvisc	0.0000173	Pa×s	562.83	Joback Method
dvisc	0.0000117	Pa×s	583.63	Joback Method
hvapt	70.50	kJ/mol	308.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3428248&Units=SI
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

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
hvapt: Enthalpy of vaporization at a given temperature
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