

4,5-Dichloro-2-methoxyphenol

Inchi:	InChI=1S/C7H6Cl2O2/c1-11-7-3-5(9)4(8)2-6(7)10/h2-3,10H,1H3
InchiKey:	HAAFFTHBNFBVKY-UHFFFAOYSA-N
Formula:	C7H6Cl2O2
SMILES:	COc1cc(Cl)c(Cl)cc1O
Mol. weight [g/mol]:	193.03

Physical Properties

Property code	Value	Unit	Source
gf	-182.27	kJ/mol	Joback Method
hf	-315.23	kJ/mol	Joback Method
hfus	22.51	kJ/mol	Joback Method
hvap	58.97	kJ/mol	Joback Method
log10ws	-2.53		Aqueous Solubility Prediction Method
logp	2.708		Crippen Method
mcvol	121.950	ml/mol	McGowan Method
pc	4266.28	kPa	Joback Method
tb	574.10	K	Joback Method
tc	813.27	K	Joback Method
tf	413.90	K	Joback Method
vc	0.402	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.37	J/molxK	574.10	Joback Method
cpg	282.31	J/molxK	773.41	Joback Method
cpg	276.01	J/molxK	733.55	Joback Method
cpg	269.33	J/molxK	693.68	Joback Method
cpg	262.19	J/molxK	653.82	Joback Method
cpg	254.56	J/molxK	613.96	Joback Method
cpg	288.27	J/molxK	813.27	Joback Method
dvisc	0.0000460	Paxs	574.10	Joback Method
dvisc	0.0000639	Paxs	547.40	Joback Method

dvisc	0.0000919	Paxs	520.70	Joback Method
dvisc	0.0001375	Paxs	494.00	Joback Method
dvisc	0.0002153	Paxs	467.30	Joback Method
dvisc	0.0003560	Paxs	440.60	Joback Method
dvisc	0.0006281	Paxs	413.90	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

cp_g:	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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ 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

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