

2-Chloro-5-methylbenzene-1,3-diol

Inchi:	InChI=1S/C7H7ClO2/c1-4-2-5(9)7(8)6(10)3-4/h2-3,9-10H,1H3
InchiKey:	HLQYXRJVJOUOMFF-UHFFFAOYSA-N
Formula:	C7H7ClO2
SMILES:	Cc1cc(O)c(Cl)c(O)c1
Mol. weight [g/mol]:	158.58
CAS:	56021-31-9

Physical Properties

Property code	Value	Unit	Source
gf	-210.33	kJ/mol	Joback Method
hf	-333.11	kJ/mol	Joback Method
hfus	23.30	kJ/mol	Joback Method
hvap	64.53	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	2.060		Crippen Method
mcvol	109.710	ml/mol	McGowan Method
pc	5800.57	kPa	Joback Method
rinpol	1439.50		NIST Webbook
rinpol	1439.50		NIST Webbook
tb	589.89	K	Joback Method
tc	838.26	K	Joback Method
tf	460.95	K	Joback Method
vc	0.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.41	J/molxK	589.89	Joback Method
cpg	253.38	J/molxK	631.28	Joback Method
cpg	260.68	J/molxK	672.68	Joback Method
cpg	267.45	J/molxK	714.07	Joback Method
cpg	273.85	J/molxK	755.47	Joback Method
cpg	280.03	J/molxK	796.86	Joback Method
cpg	286.13	J/molxK	838.26	Joback Method

dvisc	0.0001643	Paxs	460.95	Joback Method
dvisc	0.0000907	Paxs	482.44	Joback Method
dvisc	0.0000527	Paxs	503.93	Joback Method
dvisc	0.0000320	Paxs	525.42	Joback Method
dvisc	0.0000202	Paxs	546.91	Joback Method
dvisc	0.0000132	Paxs	568.40	Joback Method
dvisc	0.0000089	Paxs	589.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C56021319&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

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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