Benzaldehyde, 5-(chloromethyl)-2-hydroxy-

Other names:	2,5-Cresotaldehyde, «alpha»-chloro-
	3-Formyl-4-hydroxybenzyl chloride
	5-(Chloromethyl)salicylaldehyde
	5-(Chloromethyl)-2-hydroxybenzaldehyde
Inchi:	InChI=1S/C8H7ClO2/c9-4-6-1-2-8(11)7(3-6)5-10/h1-3,5,11H,4H2
InchiKey:	WFACWTZLXIFJCM-UHFFFAOYSA-N
Formula:	C8H7ClO2
SMILES:	O=Cc1cc(CCl)ccc1O
Mol. weight [g/mol]:	170.59
CAS:	23731-06-8

Physical Properties

Property code	Value	Unit	Source
gf	-146.81	kJ/mol	Joback Method
hf	-262.02	kJ/mol	Joback Method
hfus	22.40	kJ/mol	Joback Method
hvap	60.46	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	1.943		Crippen Method
mcvol	119.500	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
tb	580.81	K	Joback Method
tc	815.72	K	Joback Method
tf	402.50	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.87	J/mol×K	580.81	Joback Method
cpg	268.85	J/mol×K	619.96	Joback Method
cpg	277.13	J/mol×K	659.11	Joback Method
cpg	284.79	J/mol×K	698.26	Joback Method
cpg	291.93	J/mol×K	737.41	Joback Method

cpg	298.60	J/mol×K	776.57	Joback Method
cpg	304.90	J/mol×K	815.72	Joback Method
dvisc	0.0011980	Pa×s	402.50	Joback Method
dvisc	0.0006130	Pa×s	432.22	Joback Method
dvisc	0.0003419	Pa×s	461.94	Joback Method
dvisc	0.0002046	Pa×s	491.65	Joback Method
dvisc	0.0001299	Pa×s	521.37	Joback Method
dvisc	0.0000865	Pa×s	551.09	Joback Method
dvisc	0.0000601	Pa×s	580.81	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23731068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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