5-Chloro-2-hydroxy benzaldehyde

Other names: Salicylaldehyde, 5-chloro-
2-Hydroxy-5-chlorobenzaldehyde
4-Chloro-2-formylphenol
5-Chloro-2-hydroxybenzaldehyde
5-Chlorosalicylaldehyde
Benzaldehyde, 2-hydroxy, 5-chloro

Inchi: InChI=1S/C7H5ClO2/c8-6-1-2-7(10)5(3-6)4-9/h1-4,10H

InchiKey: FUGKCSRLAQKUHG-UHFFFAOYSA-N

Formula: C7H5ClO2

SMILES: O=Cc1cc(Cl)ccc1O

Mol. weight [g/mol]: 156.57

Physical Properties

Property code	Value	Unit	Source
hf	-268.51	kJ/mol	Cheméo Relay (1.0)
hfus	19.81	kJ/mol	Joback Method
hvap	64.17	kJ/mol	Cheméo Relay (1.0)
ie	8.84	eV	Cheméo Relay (1.0)
log10ws	-2.03		Cheméo Relay (1.0)
logp	1.858		Crippen Method
mcvol	105.410	ml/mol	McGowan Method
rinpol	1169.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1190.00		NIST Webbook
ripol	1966.00		NIST Webbook
ripol	1966.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1966.00		NIST Webbook
ripol	1965.00		NIST Webbook
tb	515.30	K	Cheméo Relay (1.0)

tf	332.90	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.03	J/mol×K	557.93	Joback Method
cpg	224.89	J/mol×K	597.89	Joback Method
cpg	232.07	J/mol×K	637.85	Joback Method
cpg	238.67	J/mol×K	677.81	Joback Method
cpg	244.76	J/mol×K	717.77	Joback Method
cpg	250.42	J/mol×K	757.73	Joback Method
cpg	255.74	J/mol×K	797.69	Joback Method
dvisc	0.0013964	Pa×s	391.23	Joback Method
dvisc	0.0007298	Pa×s	419.01	Joback Method
dvisc	0.0004135	Pa×s	446.80	Joback Method
dvisc	0.0002504	Pa×s	474.58	Joback Method
dvisc	0.0001603	Pa×s	502.36	Joback Method
dvisc	0.0001075	Pa×s	530.15	Joback Method
dvisc	0.0000750	Pa×s	557.93	Joback Method

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=C635938&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

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point