2,6-Dichlorobenzaldehyde

Other names: 2,6-Dichlorobenzaldehyde
Inchi: InChI=1S/C7H4Cl2O/c8-6-2-1-3-7(9)5(6)4-10/h1-4H
InchiKey: DMIYKWPEFRFTPY-UHFFFAOYSA-N
Formula: C7H4Cl2O
SMILES: O=Cc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 175.01

Physical Properties

Property code	Value	Unit	Source
af	0.4196		Cheméo Relay (1.0)
gf	-22.17	kJ/mol	Joback Method
hf	-112.89	kJ/mol	Cheméo Relay (1.0)
hfus	17.83	kJ/mol	Joback Method
hvap	59.34	kJ/mol	Cheméo Relay (1.0)
ie	9.57	eV	Cheméo Relay (1.0)
log10ws	-2.60		Cheméo Relay (1.0)
logp	2.806		Crippen Method
mcvol	111.780	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	511.58	K	Cheméo Relay (1.0)
tc	785.32	K	Cheméo Relay (1.0)
tf	343.00 ± 3.00	K	NIST Webbook
vc	0.397	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.12	J/mol×K	519.72	Joback Method
cpg	238.00	J/mol×K	753.22	Joback Method
cpg	232.58	J/mol×K	714.30	Joback Method
cpg	226.69	J/mol×K	675.39	Joback Method
cpg	220.33	J/mol×K	636.47	Joback Method
cpg	213.46	J/mol×K	597.55	Joback Method
cpg	206.07	J/mol×K	558.64	Joback Method

dvisc	0.0006513	Pa×s	420.84	Joback Method
dvisc	0.0003403	Pa×s	519.72	Joback Method
dvisc	0.0004103	Pa×s	486.76	Joback Method
dvisc	0.0005084	Pa×s	453.80	Joback Method
dvisc	0.0018573	Pa×s	321.95	Joback Method
dvisc	0.0008704	Pa×s	387.87	Joback Method
dvisc	0.0012274	Pa×s	354.91	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C83385&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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