2,3-DICHLOROBENZALDEHYDE

Other names: Benzaldehyde, 2,3-dichloro-
Inchi: InChI=1S/C7H4Cl2O/c8-6-3-1-2-5(4-10)7(6)9/h1-4H
InchiKey: LLMLNAVBOAMOEE-UHFFFAOYSA-N
Formula: C7H4Cl2O
SMILES: O=Cc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 175.01

Physical Properties

Property code	Value	Unit	Source
hf	-114.36	kJ/mol	Cheméo Relay (1.0)
hfus	17.83	kJ/mol	Joback Method
hvap	62.53	kJ/mol	Cheméo Relay (1.0)
ie	9.47	eV	Cheméo Relay (1.0)
log10ws	-2.59		Cheméo Relay (1.0)
logp	2.806		Crippen Method
mcvol	111.780	ml/mol	McGowan Method
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
tb	514.83	K	Cheméo Relay (1.0)
tf	309.57	K	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	206.07	J/mol×K	558.64	Joback Method
cpg	213.46	J/mol×K	597.55	Joback Method
cpg	220.33	J/mol×K	636.47	Joback Method
cpg	226.69	J/mol×K	675.39	Joback Method
cpg	232.58	J/mol×K	714.30	Joback Method
cpg	238.00	J/mol×K	753.22	Joback Method
dvisc	0.0018573	Pa×s	321.95	Joback Method
dvisc	0.0012274	Pa×s	354.91	Joback Method
dvisc	0.0008704	Pa×s	387.87	Joback Method

dvisc	0.0006513	Pa×s	420.84	Joback Method
dvisc	0.0005084	Pa×s	453.80	Joback Method
dvisc	0.0004103	Pa×s	486.76	Joback Method
dvisc	0.0003403	Pa×s	519.72	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6334185&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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point

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