

3,5-DICHLOROBENZALDEHYDE

Other names:	Benzaldehyde, 3,5-dichloro-
Inchi:	InChI=1S/C7H4Cl2O/c8-6-1-5(4-10)2-7(9)3-6/h1-4H
InchiKey:	CASRSOJWLARCRX-UHFFFAOYSA-N
Formula:	C7H4Cl2O
SMILES:	O=Cc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	175.01

Physical Properties

Property code	Value	Unit	Source
ea	0.99 ± 0.09	eV	NIST Webbook
ea	1.01 ± 0.09	eV	NIST Webbook
hf	-109.55	kJ/mol	Cheméo Relay (1.0)
hfus	17.83	kJ/mol	Joback Method
hvap	63.56	kJ/mol	Cheméo Relay (1.0)
ie	9.75	eV	Cheméo Relay (1.0)
log10ws	-2.73		Cheméo Relay (1.0)
logp	2.806		Crippen Method
mcvol	111.780	ml/mol	McGowan Method
tb	506.35	K	Cheméo Relay (1.0)
tf	301.56	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	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	510.70	K	99.70	NIST Webbook

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10203084&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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