

5-Chloro-1,3-benzodioxole

Other names:	1,3-Benzodioxole, 5-chloro-
Inchi:	InChI=1S/C7H5ClO2/c8-5-1-2-6-7(3-5)10-4-9-6/h1-3H,4H2
InchiKey:	ODQPZHOXLYATLC-UHFFFAOYSA-N
Formula:	C7H5ClO2
SMILES:	Clc1ccc2c(c1)OCO2
Mol. weight [g/mol]:	156.57
CAS:	7228-38-8

Physical Properties

Property code	Value	Unit	Source
gf	-14.50	kJ/mol	Joback Method
hf	-160.82	kJ/mol	Joback Method
hfus	24.37	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.069		Crippen Method
mcvol	98.850	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
tb	459.20	K	NIST Webbook
tc	737.80	K	Joback Method
tf	325.35	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.14	J/mol×K	498.94	Joback Method
cpg	237.92	J/mol×K	697.99	Joback Method
cpg	231.11	J/mol×K	658.18	Joback Method
cpg	223.69	J/mol×K	618.37	Joback Method
cpg	215.60	J/mol×K	578.56	Joback Method
cpg	206.77	J/mol×K	538.75	Joback Method
cpg	244.18	J/mol×K	737.80	Joback Method
dvisc	0.0005441	Pa×s	498.94	Joback Method

dvisc	0.0006354	Pa×s	470.01	Joback Method
dvisc	0.0007572	Pa×s	441.08	Joback Method
dvisc	0.0009250	Pa×s	412.14	Joback Method
dvisc	0.0011646	Pa×s	383.21	Joback Method
dvisc	0.0015224	Pa×s	354.28	Joback Method
dvisc	0.0020874	Pa×s	325.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7228388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
mccvol:	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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