1,2-Dimethoxy-4-chloro-benzene

Other names:	4-Chloroveratrole
	4-Chloro-1,2-dimethoxybenzene
	4-Chloro-2-methoxyphenol, methyl ether
	Benzene, 4-chloro-1,2-dimethoxy
Inchi:	InChI=1S/C8H9ClO2/c1-10-7-4-3-6(9)5-8(7)11-2/h3-5H,1-2H3
InchiKey:	RXJCXGJKJZARAW-UHFFFAOYSA-N
Formula:	C8H9ClO2
SMILES:	COc1ccc(Cl)cc1OC
Mol. weight [g/mol]:	172.61
CAS:	16766-27-1

Physical Properties

Property code	Value	Unit	Source
gf	-112.30	kJ/mol	Joback Method
hf	-275.04	kJ/mol	Joback Method
hfus	16.31	kJ/mol	Joback Method
hvap	46.21	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.357		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1335.30		NIST Webbook
ripol	1959.00		NIST Webbook
ripol	1975.00		NIST Webbook
ripol	1994.00		NIST Webbook
ripol	1959.00		NIST Webbook
ripol	1951.00		NIST Webbook
tb	501.35	K	Joback Method
tc	716.87	K	Joback Method
tf	305.76	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.94	J/mol×K	501.35	Joback Method
cpg	256.80	J/mol×K	537.27	Joback Method
cpg	267.21	J/mol×K	573.19	Joback Method
cpg	277.16	J/mol×K	609.11	Joback Method
cpg	286.64	J/mol×K	645.03	Joback Method
cpg	295.64	J/mol×K	680.95	Joback Method
cpg	304.15	J/mol×K	716.87	Joback Method
dvisc	0.0010775	Pa×s	305.76	Joback Method
dvisc	0.0006910	Pa×s	338.36	Joback Method
dvisc	0.0004791	Pa×s	370.96	Joback Method
dvisc	0.0003524	Pa×s	403.56	Joback Method
dvisc	0.0002714	Pa×s	436.15	Joback Method
dvisc	0.0002168	Pa×s	468.75	Joback Method
dvisc	0.0001783	Pa×s	501.35	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16766271&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume