1,2-Dimethoxy-3,6-dichloro-benzene

Other names: Benzene, 3,6-dichloro-1,2-dimethoxy
Inchi: InChI=1S/C8H8Cl2O2/c1-11-7-5(9)3-4-6(10)8(7)12-2/h3-4H,1-2H3
InchiKey: CBYMFVMZRAOHOY-UHFFFAOYSA-N
Formula: C8H8Cl2O2
SMILES: COc1c(Cl)ccc(Cl)c1OC
Mol. weight [g/mol]: 207.05
CAS: 90283-02-6

Physical Properties

Property code	Value	Unit	Source
gf	-133.86	kJ/mol	Joback Method
hf	-302.25	kJ/mol	Joback Method
hfus	20.12	kJ/mol	Joback Method
hvap	51.25	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	3.011		Crippen Method
mcvol	136.040	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
rinpol	1343.00		NIST Webbook
rinpol	1342.00		NIST Webbook
rinpol	1371.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1340.00		NIST Webbook
ripol	1864.00		NIST Webbook
ripol	1864.00		NIST Webbook
ripol	1886.00		NIST Webbook
ripol	1916.00		NIST Webbook
ripol	1870.00		NIST Webbook
ripol	1870.00		NIST Webbook
tb	543.76	K	Joback Method
tc	765.36	K	Joback Method
tf	348.20	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.48	J/mol×K	543.76	Joback Method
cpg	314.19	J/mol×K	728.42	Joback Method
cpg	305.98	J/mol×K	691.49	Joback Method
cpg	297.29	J/mol×K	654.56	Joback Method
cpg	288.14	J/mol×K	617.63	Joback Method
cpg	278.53	J/mol×K	580.69	Joback Method
cpg	321.89	J/mol×K	765.36	Joback Method
dvisc	0.0001753	Pa×s	543.76	Joback Method
dvisc	0.0002098	Pa×s	511.17	Joback Method
dvisc	0.0002572	Pa×s	478.57	Joback Method
dvisc	0.0003249	Pa×s	445.98	Joback Method
dvisc	0.0004258	Pa×s	413.39	Joback Method
dvisc	0.0005846	Pa×s	380.79	Joback Method
dvisc	0.0008515	Pa×s	348.20	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C90283026&Units=SI

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