1,2-DIMETHOXY-3,4-DICHLORO-BENZENE

Other names: Benzene, 3,4-dichloro-1,2-dimethoxy
Inchi: InChI=1S/C8H8Cl2O2/c1-11-6-4-3-5(9)7(10)8(6)12-2/h3-4H,1-2H3
InchiKey: WEMHPBMPYVGSJI-UHFFFAOYSA-N
Formula: C8H8Cl2O2
SMILES: COc1ccc(Cl)c(Cl)c1OC
Mol. weight [g/mol]: 207.06

Physical Properties

Property code	Value	Unit	Source
hf	-268.39	kJ/mol	Cheméo Relay (1.0)
hfus	20.12	kJ/mol	Joback Method
hvap	70.73	kJ/mol	Cheméo Relay (1.0)
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-3.22		Cheméo Relay (1.0)
logp	3.011		Crippen Method
mcvol	136.040	ml/mol	McGowan Method
rinpol	1455.00		NIST Webbook
rinpol	1448.00		NIST Webbook
rinpol	1451.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1461.00		NIST Webbook
ripol	2108.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2150.00		NIST Webbook
ripol	2171.00		NIST Webbook
ripol	2134.00		NIST Webbook
tb	533.55	K	Cheméo Relay (1.0)
tf	328.70	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.48	J/mol×K	543.76	Joback Method
cpg	321.89	J/mol×K	765.36	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
dvisc	0.0003249	Pa×s	445.98	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	0.0008515	Pa×s	348.20	Joback Method
dvisc	0.0004258	Pa×s	413.39	Joback Method
dvisc	0.0005846	Pa×s	380.79	Joback Method

Sources

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=C90283004&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

ripol: Polar retention indices

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point