1,2-DIMETHOXY-4,5-DICHLORO-BENZENE

Other names: 4,5-Dichloroveratrole
Benzene, 4,5-dichloro-1,2-dimethoxy
Inchi: InChI=1S/C8H8Cl2O2/c1-11-7-3-5(9)6(10)4-8(7)12-2/h3-4H,1-2H3
InchiKey: RJYXLZQZBLGBOM-UHFFFAOYSA-N
Formula: C8H8Cl2O2
SMILES: COc1cc(Cl)c(Cl)cc1OC
Mol. weight [g/mol]: 207.06

Physical Properties

Property code	Value	Unit	Source
hf	-282.91	kJ/mol	Cheméo Relay (1.0)
hfus	20.12	kJ/mol	Joback Method
hvap	71.27	kJ/mol	Cheméo Relay (1.0)
ie	8.19	eV	Cheméo Relay (1.0)
log10ws	-3.46		Aqueous Solubility Prediction Method
logp	3.011		Crippen Method
mcvol	136.040	ml/mol	McGowan Method
rinpol	1503.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1484.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1484.00		NIST Webbook
ripol	2213.00		NIST Webbook
ripol	2228.00		NIST Webbook
ripol	2216.00		NIST Webbook
ripol	2203.00		NIST Webbook
ripol	2188.00		NIST Webbook
tb	536.31	K	Cheméo Relay (1.0)
tf	380.47	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	278.53	J/mol×K	580.69	Joback Method
cpg	288.14	J/mol×K	617.63	Joback Method
cpg	297.29	J/mol×K	654.56	Joback Method
cpg	305.98	J/mol×K	691.49	Joback Method
cpg	314.19	J/mol×K	728.42	Joback Method
cpg	321.89	J/mol×K	765.36	Joback Method
dvisc	0.0008515	Pa×s	348.20	Joback Method
dvisc	0.0005846	Pa×s	380.79	Joback Method
dvisc	0.0004258	Pa×s	413.39	Joback Method
dvisc	0.0003249	Pa×s	445.98	Joback Method
dvisc	0.0002572	Pa×s	478.57	Joback Method
dvisc	0.0002098	Pa×s	511.17	Joback Method
dvisc	0.0001753	Pa×s	543.76	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2772465&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