1,2-Dimethoxy-3,4,6-trichloro-benzene

Other names: Benzene, 3,4,6-trichloro-1,2-dimethoxy
Inchi: InChI=1S/C8H7Cl3O2/c1-12-7-5(10)3-4(9)6(11)8(7)13-2/h3H,1-2H3
InchiKey: BGWJOOFPIQFVOT-UHFFFAOYSA-N
Formula: C8H7Cl3O2
SMILES: COc1c(Cl)cc(Cl)c(Cl)c1OC
Mol. weight [g/mol]: 241.50
CAS: 85298-07-3

Physical Properties

Property code	Value	Unit	Source
gf	-155.42	kJ/mol	Joback Method
hf	-329.46	kJ/mol	Joback Method
hfus	23.93	kJ/mol	Joback Method
hvap	56.30	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.664		Crippen Method
mcvol	148.280	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1536.00		NIST Webbook
ripol	2058.00		NIST Webbook
ripol	2034.00		NIST Webbook
ripol	2060.00		NIST Webbook
ripol	2088.00		NIST Webbook
tb	586.17	K	Joback Method
tc	812.98	K	Joback Method
tf	390.64	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.10	J/mol×K	586.17	Joback Method
cpg	298.34	J/mol×K	623.97	Joback Method
cpg	307.16	J/mol×K	661.77	Joback Method
cpg	315.53	J/mol×K	699.57	Joback Method
cpg	323.42	J/mol×K	737.38	Joback Method
cpg	330.81	J/mol×K	775.18	Joback Method
cpg	337.68	J/mol×K	812.98	Joback Method
dvisc	0.0006860	Pa×s	390.64	Joback Method
dvisc	0.0004955	Pa×s	423.23	Joback Method
dvisc	0.0003749	Pa×s	455.82	Joback Method
dvisc	0.0002945	Pa×s	488.41	Joback Method
dvisc	0.0002384	Pa×s	520.99	Joback Method
dvisc	0.0001978	Pa×s	553.58	Joback Method
dvisc	0.0001676	Pa×s	586.17	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85298073&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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