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

Physical Properties

Property code	Value	Unit	Source
hf	-263.18	kJ/mol	Cheméo Relay (1.0)
hfus	23.93	kJ/mol	Joback Method
hvap	74.64	kJ/mol	Cheméo Relay (1.0)
ie	8.31	eV	Cheméo Relay (1.0)
log10ws	-4.10		Cheméo Relay (1.0)
logp	3.664		Crippen Method
mcvol	148.280	ml/mol	McGowan Method
rinpol	1511.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
ripol	2058.00		NIST Webbook
ripol	2088.00		NIST Webbook
ripol	2060.00		NIST Webbook
ripol	2034.00		NIST Webbook
tb	542.35	K	Cheméo Relay (1.0)
tf	342.77	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85298073&Units=SI

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

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

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):

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