

1,2-Dimethoxy-3-chloro-benzene

Other names:	3-Chloroveratrole Benzene, 3-chloro-1,2-dimethoxy
Inchi:	InChI=1S/C8H9ClO2/c1-10-7-5-3-4-6(9)8(7)11-2/h3-5H,1-2H3
InchiKey:	JVCXXMPHTZGGNV-UHFFFAOYSA-N
Formula:	C8H9ClO2
SMILES:	COc1cccc(Cl)c1OC
Mol. weight [g/mol]:	172.61
CAS:	90282-99-8

Physical Properties

Property code	Value	Unit	Source
gf	-112.30	kJ/mol	Joback Method
hf	-275.04	kJ/mol	Joback Method
hfus	16.31	kJ/mol	Joback Method
hvap	46.21	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.357		Crippen Method
mcvol	123.800	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
ripol	1263.00		NIST Webbook
ripol	1263.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1262.00		NIST Webbook
ripol	1281.00		NIST Webbook
ripol	1266.00		NIST Webbook
ripol	1263.00		NIST Webbook
ripol	1847.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1883.00		NIST Webbook
ripol	1851.00		NIST Webbook
tb	501.35	K	Joback Method
tc	716.87	K	Joback Method
tf	305.76	K	Joback Method
vc	0.461	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.94	J/molxK	501.35	Joback Method
cpg	256.80	J/molxK	537.27	Joback Method
cpg	267.21	J/molxK	573.19	Joback Method
cpg	277.16	J/molxK	609.11	Joback Method
cpg	286.64	J/molxK	645.03	Joback Method
cpg	295.64	J/molxK	680.95	Joback Method
cpg	304.15	J/molxK	716.87	Joback Method
dvisc	0.0010775	Paxs	305.76	Joback Method
dvisc	0.0006910	Paxs	338.36	Joback Method
dvisc	0.0004791	Paxs	370.96	Joback Method
dvisc	0.0003524	Paxs	403.56	Joback Method
dvisc	0.0002714	Paxs	436.15	Joback Method
dvisc	0.0002168	Paxs	468.75	Joback Method
dvisc	0.0001783	Paxs	501.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90282998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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