

1,2-DIMETHOXY-3,5-DICHLORO-BENZENE

Other names: Benzene, 3,5-dichloro-1,2-dimethoxy

Inchi: InChI=1S/C8H8Cl2O2/c1-11-7-4-5(9)3-6(10)8(7)12-2/h3-4H,1-2H3

InchiKey: BCWABYVHGXOWHB-UHFFFAOYSA-N

Formula: C8H8Cl2O2

SMILES: COc1cc(Cl)cc(Cl)c1OC

Mol. weight [g/mol]: 207.06

Physical Properties

Property code	Value	Unit	Source
hfus	20.12	kJ/mol	Joback Method
log10ws	-3.28		Cheméo Relay (1.0)
logp	3.011		Crippen Method
mcvol	136.040	ml/mol	McGowan Method
rinpol	1419.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1414.00	NIST Webbook	NIST Webbook
rinpol	1436.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1410.00	NIST Webbook	NIST Webbook
ripol	2009.00		NIST Webbook
ripol	2025.00		NIST Webbook
ripol	2045.00	NIST Webbook	NIST Webbook
ripol	2067.00		NIST Webbook
ripol	2023.00		NIST Webbook
tf	329.20	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		580.69	Joback Method
cpg	288.14		617.63	Joback Method
cpg	297.29		654.56	Joback Method
cpg	305.98		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90283015&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):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
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
tf:	Normal melting (fusion) point

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