

Benzene, 1,3-dichloro-2-(dichloromethyl)-

Other names:	Toluene, «alpha», «alpha»2,6-tetrachloro- «alpha», «alpha», 2,6-Tetrachlorotoluene 2,6-Dichlorobenzal chloride 2,6-Dichlorobenzylidene chloride Benzene, 2,6-dichloro-1-(dichloromethyl)
Inchi:	InChI=1S/C7H4Cl4/c8-4-2-1-3-5(9)6(4)7(10)11/h1-3,7H
InchiKey:	QQPXXHAEIGVZKQ-UHFFFAOYSA-N
Formula:	C7H4Cl4
SMILES:	Clc1cccc(Cl)c1C(Cl)Cl
Mol. weight [g/mol]:	229.92
CAS:	81-19-6

Physical Properties

Property code	Value	Unit	Source
gf	51.05	kJ/mol	Joback Method
hf	-42.46	kJ/mol	Joback Method
hfus	20.41	kJ/mol	Joback Method
hvap	51.93	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	4.470		Crippen Method
mcvol	134.690	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	545.48	K	Joback Method
tc	790.96	K	Joback Method
tf	324.79	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.70	J/molxK	545.48	Joback Method
cpg	236.90	J/molxK	586.39	Joback Method
cpg	244.46	J/molxK	627.31	Joback Method
cpg	251.40	J/molxK	668.22	Joback Method

cpg	257.78	J/molxK	709.13	Joback Method
cpg	263.61	J/molxK	750.05	Joback Method
cpg	268.93	J/molxK	790.96	Joback Method
dvisc	0.0020204	Paxs	324.79	Joback Method
dvisc	0.0012150	Paxs	361.57	Joback Method
dvisc	0.0008027	Paxs	398.35	Joback Method
dvisc	0.0005687	Paxs	435.13	Joback Method
dvisc	0.0004252	Paxs	471.92	Joback Method
dvisc	0.0003316	Paxs	508.70	Joback Method
dvisc	0.0002674	Paxs	545.48	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81196&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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