

2,4,4'-trichlorodiphenyl ether

Inchi:	InChI=1S/C12H7Cl3O/c13-8-1-4-10(5-2-8)16-12-6-3-9(14)7-11(12)15/h1-7H
InchiKey:	PIORTDHJOLELKR-UHFFFAOYSA-N
Formula:	C12H7Cl3O
SMILES:	Clc1ccc(Oc2ccc(Cl)cc2Cl)cc1
Mol. weight [g/mol]:	273.55

Physical Properties

Property code	Value	Unit	Source
gf	105.30	kJ/mol	Joback Method
hf	-31.80	kJ/mol	Joback Method
hfus	27.53	kJ/mol	Joback Method
hvap	64.41	kJ/mol	Joback Method
log10ws	-6.22		Aqueous Solubility Prediction Method
logp	5.439		Crippen Method
mcvol	175.010	ml/mol	McGowan Method
pc	2826.33	kPa	Joback Method
tb	676.97	K	Joback Method
tc	935.56	K	Joback Method
tf	427.39	K	Joback Method
vc	0.656	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.90	J/mol×K	676.97	Joback Method
cpg	419.81	J/mol×K	892.46	Joback Method
cpg	412.06	J/mol×K	849.36	Joback Method
cpg	403.43	J/mol×K	806.27	Joback Method
cpg	393.89	J/mol×K	763.17	Joback Method
cpg	383.39	J/mol×K	720.07	Joback Method
cpg	426.71	J/mol×K	935.56	Joback Method
dvisc	0.0001457	Paxs	676.97	Joback Method
dvisc	0.0001766	Paxs	635.37	Joback Method

dvisc	0.0002200	Paxs	593.78	Joback Method
dvisc	0.0002831	Paxs	552.18	Joback Method
dvisc	0.0003797	Paxs	510.58	Joback Method
dvisc	0.0005365	Paxs	468.99	Joback Method
dvisc	0.0008107	Paxs	427.39	Joback Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method:

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

Aqueous Solubility Prediction Method:

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

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

Latest version available from:

<https://www.cheméo.com/cid/101-102-5/2-4-4-trichlorodiphenyl-ether.pdf>

Generated by Cheméo on 2026-05-18 12:24:20.751855427 +0000 UTC m=+2872409.809937652.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.