

3,3',4,4'-tetrachlorodiphenyl ether

Inchi:	InChI=1S/C12H6Cl4O/c13-9-3-1-7(5-11(9)15)17-8-2-4-10(14)12(16)6-8/h1-6H
InchiKey:	DHLVZXZRIZBPKG-UHFFFAOYSA-N
Formula:	C12H6Cl4O
SMILES:	Clc1ccc(Oc2ccc(Cl)c(Cl)c2)cc1Cl
Mol. weight [g/mol]:	307.99

Physical Properties

Property code	Value	Unit	Source
gf	83.74	kJ/mol	Joback Method
hf	-59.01	kJ/mol	Joback Method
hfus	31.34	kJ/mol	Joback Method
hvap	69.46	kJ/mol	Joback Method
log10ws	-6.98		Aqueous Solubility Prediction Method
logp	6.092		Crippen Method
mcvol	187.250	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
tb	719.38	K	Joback Method
tc	980.81	K	Joback Method
tf	469.83	K	Joback Method
vc	0.706	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.71	J/molxK	719.38	Joback Method
cpg	400.91	J/molxK	762.95	Joback Method
cpg	410.17	J/molxK	806.52	Joback Method
cpg	418.52	J/molxK	850.09	Joback Method
cpg	426.00	J/molxK	893.66	Joback Method
cpg	432.64	J/molxK	937.23	Joback Method
cpg	438.47	J/molxK	980.81	Joback Method
dvisc	0.0006337	Paxs	469.83	Joback Method
dvisc	0.0004398	Paxs	511.42	Joback Method

dvisc	0.0003225	Paxs	553.01	Joback Method
dvisc	0.0002470	Paxs	594.61	Joback Method
dvisc	0.0001959	Paxs	636.20	Joback Method
dvisc	0.0001598	Paxs	677.79	Joback Method
dvisc	0.0001335	Paxs	719.38	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

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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