2,4,5-trichlorodiphenyl ether

Inchi: InChI=1S/C12H7Cl3O/c13-9-6-11(15)12(7-10(9)14)16-8-4-2-1-3-5-8/h1-7H
InchiKey: UWKZWXCTDPYXHU-UHFFFAOYSA-N
Formula: C12H7Cl3O
SMILES: Clc1cc(Cl)c(Oc2ccccc2)cc1Cl
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	-6.58		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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.90	J/mol×K	676.97	Joback Method
cpg	383.39	J/mol×K	720.07	Joback Method
cpg	393.89	J/mol×K	763.17	Joback Method
cpg	403.43	J/mol×K	806.27	Joback Method
cpg	412.06	J/mol×K	849.36	Joback Method
cpg	419.81	J/mol×K	892.46	Joback Method
cpg	426.71	J/mol×K	935.56	Joback Method
dvisc	0.0008107	Pa×s	427.39	Joback Method
dvisc	0.0005365	Pa×s	468.99	Joback Method

dvisc	0.0003797	Pa×s	510.58	Joback Method
dvisc	0.0002831	Pa×s	552.18	Joback Method
dvisc	0.0002200	Pa×s	593.78	Joback Method
dvisc	0.0001766	Pa×s	635.37	Joback Method
dvisc	0.0001457	Pa×s	676.97	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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