Diphenylsulfone, 4-chloro-4'-methyl-

Other names: 4-Methyl-4'-chlorodiphenylsulfone
Inchi: InChI=1S/C13H11ClO2S/c1-10-2-6-12(7-3-10)17(15,16)13-8-4-11(14)5-9-13/h2-9H,1H3
InchiKey: OFGLBHMUHZRKFN-UHFFFAOYSA-N
Formula: C13H11ClO2S
SMILES: Cc1ccc(S(=O)(=O)c2ccc(Cl)cc2)cc1
Mol. weight [g/mol]: 266.74
CAS: 5184-71-4

Physical Properties

Property code	Value	Unit	Source
gf	-216.33	kJ/mol	Joback Method
hf	-330.62	kJ/mol	Joback Method
hfus	32.30	kJ/mol	Joback Method
hvap	73.43	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.481		Crippen Method
mcvol	186.840	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
tb	645.37	K	Joback Method
tc	884.05	K	Joback Method
tf	382.63	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.28	J/mol×K	645.37	Joback Method
cpg	447.96	J/mol×K	685.15	Joback Method
cpg	461.42	J/mol×K	724.93	Joback Method
cpg	473.72	J/mol×K	764.71	Joback Method
cpg	484.88	J/mol×K	804.49	Joback Method
cpg	494.95	J/mol×K	844.27	Joback Method
cpg	503.94	J/mol×K	884.05	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=C5184714&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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