

Phenol, 2,2'-sulfinylbis[4-chloro-

Other names:	2,2'-Sulfinylbis(4-chlorophenol)
Inchi:	InChI=1S/C12H8Cl2O3S/c13-7-1-3-9(15)11(5-7)18(17)12-6-8(14)2-4-10(12)16/h1-6,15-1
InchiKey:	RTKDHPNYIPCHSF-UHFFFAOYSA-N
Formula:	C12H8Cl2O3S
SMILES:	O=S(c1cc(Cl)ccc1O)c1cc(Cl)ccc1O
Mol. weight [g/mol]:	303.16
CAS:	29097-31-2

Physical Properties

Property code	Value	Unit	Source
gf	-295.09	kJ/mol	Joback Method
hf	-432.73	kJ/mol	Joback Method
hfus	41.85	kJ/mol	Joback Method
hvap	95.71	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.571		Crippen Method
mcvol	190.860	ml/mol	McGowan Method
pc	4903.92	kPa	Joback Method
tb	831.66	K	Joback Method
tc	1104.24	K	Joback Method
tf	622.64	K	Joback Method
vc	0.612	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.29	J/molxK	831.66	Joback Method
cpg	479.83	J/molxK	877.09	Joback Method
cpg	489.04	J/molxK	922.52	Joback Method
cpg	498.13	J/molxK	967.95	Joback Method
cpg	507.30	J/molxK	1013.38	Joback Method
cpg	516.77	J/molxK	1058.81	Joback Method
cpg	526.75	J/molxK	1104.24	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=C29097312&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

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