

# 2,2'-Thiobis(4-chloro-6-cyclohexylphenol)

<b>Inchi:</b>	InChI=1S/C24H28Cl2O2S/c25-17-11-19(15-7-3-1-4-8-15)23(27)21(13-17)29-22-14-18(2
<b>InchiKey:</b>	AEOOLMQCAIHHCZ-UHFFFAOYSA-N
<b>Formula:</b>	C24H28Cl2O2S
<b>SMILES:</b>	Oc1c(Sc2cc(Cl)cc(C3CCCCC3)c2O)cc(Cl)cc1C1CCCCC1
<b>Mol. weight [g/mol]:</b>	451.45
<b>CAS:</b>	116277-94-2

## Physical Properties

Property code	Value	Unit	Source
gf	86.42	kJ/mol	Joback Method
hf	-347.10	kJ/mol	Joback Method
hfus	52.20	kJ/mol	Joback Method
hvap	118.69	kJ/mol	Joback Method
log10ws	-9.02		Crippen Method
logp	8.651		Crippen Method
mcvol	332.350	ml/mol	McGowan Method
pc	1942.37	kPa	Joback Method
tb	1165.78	K	Joback Method
tc	1457.40	K	Joback Method
tf	795.60	K	Joback Method
vc	1.113	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1136.77	J/molxK	1165.78	Joback Method
cpg	1156.82	J/molxK	1214.38	Joback Method
cpg	1177.22	J/molxK	1262.99	Joback Method
cpg	1198.33	J/molxK	1311.59	Joback Method
cpg	1220.49	J/molxK	1360.19	Joback Method
cpg	1244.04	J/molxK	1408.79	Joback Method
cpg	1269.34	J/molxK	1457.40	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116277942&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116277942&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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