

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

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

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=C116277942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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