4,4'-DICHLORODIPHENYLSULPHIDE

Other names:	Sulfide, bis(p-chlorophenyl)
	p-Chlorophenyl sulfide
	Bis(p-chlorophenyl) sulfide
	Bis(4-chlorophenyl) sulfide
	Di-p-chlorophenyl sulfide
	4,4'-Dichlorodiphenyl sulfide
	Benzene, 1,1'-thiobis(4-chloro-
	4-Chlorophenyl sulfide
	NSC 40470
Inchi:	InChI=1S/C12H8Cl2S/c13-9-1-5-11(6-2-9)15-12-7-3-10(14)4-8-12/h1-8H
InchiKey:	MJEPOVIWHVRBIT-UHFFFAOYSA-N
Formula:	C12H8Cl2S
SMILES:	Clc1ccc(Sc2ccc(Cl)cc2)cc1
Mol. weight [g/mol]:	255.17

Physical Properties

Property code	Value	Unit	Source
hf	146.52	kJ/mol	Cheméo Relay (1.0)
hfus	26.66	kJ/mol	Joback Method
hvap	85.55	kJ/mol	Cheméo Relay (1.0)
ie	8.13	eV	NIST Webbook
log10ws	-6.73		Cheméo Relay (1.0)
logp	5.145		Crippen Method
mcvol	173.250	ml/mol	McGowan Method
tb	623.64	K	Cheméo Relay (1.0)
tc	840.36	K	Cheméo Relay (1.0)
tf	384.55	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.16	J/mol×K	680.92	Joback Method
cpg	386.80	J/mol×K	727.27	Joback Method
cpg	398.19	J/mol×K	773.62	Joback Method

cpg	408.42	J/mol×K	819.98	Joback Method
cpg	417.55	J/mol×K	866.33	Joback Method
cpg	425.66	J/mol×K	912.68	Joback Method
cpg	432.82	J/mol×K	959.03	Joback Method

Sources

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5181102&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point