

Benzene, 1,1'-sulfinylbis[4-chloro-

Other names:	Benzene, 1,1'-sulfinylbis[4-chloro- p-Chlorophenyl sulfoxide p,p'-Dichlorodiphenyl sulfoxide Bis(p-chlorophenyl) sulfoxide Bis(4-chlorophenyl) sulfoxide Di-p-chlorophenyl sulfoxide 4,4'-Dichlorodiphenyl sulfoxide 4,4-Dichlorodiphenyl sulfoxide Sulfoxide, bis(4-chlorophenyl)- NSC 406205 4-Chlorophenyl sulfoxide bis(p-chlorophenyl)sulphoxide
Inchi:	InChI=1S/C12H8Cl2OS/c13-9-1-5-11(6-2-9)16(15)12-7-3-10(14)4-8-12/h1-8H
InchiKey:	KJGYFISADIZFEL-UHFFFAOYSA-N
Formula:	C12H8Cl2OS
SMILES:	O=S(c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]:	271.17

Physical Properties

Property code	Value	Unit	Source
hf	17.73	kJ/mol	Cheméo Relay (1.0)
hfus	30.29	kJ/mol	Joback Method
hvap	110.99	kJ/mol	Cheméo Relay (1.0)
ie	8.70	eV	Cheméo Relay (1.0)
log10ws	-5.30		Cheméo Relay (1.0)
logp	4.160		Crippen Method
mcvol	179.120	ml/mol	McGowan Method
tb	644.75	K	Cheméo Relay (1.0)
tf	409.94	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.42	J/mol×K	670.42	Joback Method

cpg	404.14	J/mol×K	714.06	Joback Method
cpg	415.63	J/mol×K	757.69	Joback Method
cpg	425.96	J/mol×K	801.33	Joback Method
cpg	435.18	J/mol×K	844.97	Joback Method
cpg	443.35	J/mol×K	888.60	Joback Method
cpg	450.50	J/mol×K	932.24	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C3085425&Units=SI>

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

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

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
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
tf:	Normal melting (fusion) point

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