Benzene, 1,2,4-trichloro-5-[(4-chlorophenyl)sulfinyl]-

Other names: Benzene, 1,2,4-trichloro-5-[(4-chlorophenyl)sulfinyl]-
p-Chlorophenyl 2,4,5-trichlorophenyl sulfoxide
V 110

Inchi: InChI=1S/C12H6Cl4OS/c13-7-1-3-8(4-2-7)18(17)12-6-10(15)9(14)5-11(12)16/h1-6H

InchiKey: IEPUYXNXNXZXRP-UHFFFAOYSA-N

Formula: C12H6Cl4OS

SMILES: O=S(c1ccc(Cl)cc1)c1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 340.06

Physical Properties

Property code	Value	Unit	Source
hfus	37.90	kJ/mol	Joback Method
logp	5.467		Crippen Method
mcvol	203.600	ml/mol	McGowan Method
tf	415.50 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.30	J/mol×K	755.24	Joback Method
cpg	439.09	J/mol×K	799.74	Joback Method
cpg	447.79	J/mol×K	844.25	Joback Method
cpg	455.43	J/mol×K	888.75	Joback Method
cpg	462.07	J/mol×K	933.25	Joback Method
cpg	467.72	J/mol×K	977.75	Joback Method
cpg	472.45	J/mol×K	1022.26	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35850294&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
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point