Tetrasul

Other names:	Benzene, 1,2,4-trichloro-5-[(4-chlorophenyl)thio]-
	Sulfide, p-chlorophenyl 2,4,5-trichlorophenyl
	p-Chlorophenyl 2,4,5-trichlorophenyl sulfide
	Animert
	Animert V-10
	Animert V-10K
	Animert V-101
	V 101
	2,4,4',5-Tetrachlorodiphenyl sulphide
	4-Chlorophenyl 2,4,5-trichlorophenyl sulfide
	ENT 27,115
	Philips-duphar V-101
	3,4,6,4'-Tetrachlor-diphenylsulfid
	2,4,5,4'-Tetrachlorodiphenyl sulfide
	1,2,4-Trichloro-5-(4-(chlorophenyl)thio)benzene
Inchi:	InChI=1S/C12H6Cl4S/c13-7-1-3-8(4-2-7)17-12-6-10(15)9(14)5-11(12)16/h1-6H
InchiKey:	QUWSDLYBOVGOCW-UHFFFAOYSA-N
Formula:	C12H6Cl4S
SMILES:	Clc1ccc(Sc2cc(Cl)c(Cl)cc2Cl)cc1
Mol. weight [g/mol]:	324.05
CAS:	2227-13-6

Physical Properties

Property code	Value	Unit	Source
gf	221.86	kJ/mol	Joback Method
hf	115.08	kJ/mol	Joback Method
hfus	34.28	kJ/mol	Joback Method
hvap	73.86	kJ/mol	Joback Method
log10ws	-6.63		Crippen Method
logp	6.451		Crippen Method
mcvol	197.730	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
tb	765.74	K	Joback Method
tc	1048.09	K	Joback Method
tf	482.00	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.43	J/mol×K	765.74	Joback Method
cpg	420.17	J/mol×K	812.80	Joback Method
cpg	428.84	J/mol×K	859.86	Joback Method
cpg	436.50	J/mol×K	906.91	Joback Method
cpg	443.20	J/mol×K	953.97	Joback Method
cpg	449.00	J/mol×K	1001.03	Joback Method
cpg	453.96	J/mol×K	1048.09	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=C2227136&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