Bis(3,4-dichlorophenylthio)methane

Other names: Methane, bis(3,4-dichlorophenylthio)-
Inchi: InChI=1S/C13H8Cl4S2/c14-10-3-1-8(5-12(10)16)18-7-19-9-2-4-11(15)13(17)6-9/h1-6H,7
InchiKey: PVURINFQLWSBRK-UHFFFAOYSA-N
Formula: C13H8Cl4S2
SMILES: Clc1ccc(SCSc2ccc(Cl)c(Cl)c2)cc1Cl
Mol. weight [g/mol]: 370.14
CAS: 106241-40-1

Physical Properties

Property code	Value	Unit	Source
gf	263.40	kJ/mol	Joback Method
hf	136.31	kJ/mol	Joback Method
hfus	41.00	kJ/mol	Joback Method
hvap	82.91	kJ/mol	Joback Method
log10ws	-7.42		Crippen Method
logp	7.142		Crippen Method
mcvol	228.170	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
tb	857.40	K	Joback Method
tc	1146.65	K	Joback Method
tf	527.67	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.41	J/mol×K	857.40	Joback Method
cpg	512.63	J/mol×K	905.61	Joback Method
cpg	520.59	J/mol×K	953.82	Joback Method
cpg	527.32	J/mol×K	1002.03	Joback Method
cpg	532.89	J/mol×K	1050.23	Joback Method
cpg	537.33	J/mol×K	1098.44	Joback Method
cpg	540.72	J/mol×K	1146.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106241401&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
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

Latest version available from:
https://www.chemeo.com/cid/28-091-0/Bis-3-4-dichlorophenylthio-methane.pdf
Generated by Cheméo on 2024-04-29 17:58:39.702050841 +0000 UTC m=+16702768.622628153.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.