1,4-Dithiin, 2,5-bis(4-chlorophenyl)-

Other names: p-Dithiin, 2,5-bis(p-chlorophenyl)-
Inchi: InChI=1S/C16H10Cl2S2/c17-13-5-1-11(2-6-13)15-9-20-16(10-19-15)12-3-7-14(18)8-4-12
InchiKey: YEISRKIONCELHP-UHFFFAOYSA-N
Formula: C16H10Cl2S2
SMILES: Clc1ccc(C2=CSC(c3ccc(Cl)cc3)=CS2)cc1
Mol. weight [g/mol]: 337.29
CAS: 2244-77-1

Physical Properties

Property code	Value	Unit	Source
gf	418.08	kJ/mol	Joback Method
hf	302.87	kJ/mol	Joback Method
hfus	32.64	kJ/mol	Joback Method
hvap	80.13	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	6.770		Crippen Method
mcvol	226.500	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	360.90		NIST Webbook
rinpol	360.90		NIST Webbook
tb	831.82	K	Joback Method
tc	1135.18	K	Joback Method
tf	612.88	K	Joback Method
vc	0.811	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.14	J/mol×K	831.82	Joback Method
cpg	555.91	J/mol×K	882.38	Joback Method
cpg	567.31	J/mol×K	932.94	Joback Method
cpg	577.50	J/mol×K	983.50	Joback Method
cpg	586.65	J/mol×K	1034.06	Joback Method
cpg	594.93	J/mol×K	1084.62	Joback Method

cpg	602.49	J/mol×K	1135.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2244771&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume