Bis(4-chlorothiophenyl)oxalate

Inchi: InChI=1S/C14H8Cl2O2S2/c15-9-1-5-11(6-2-9)19-13(17)14(18)20-12-7-3-10(16)4-8-12/h1
InchiKey: NDEFWMFSVXHDCR-UHFFFAOYSA-N
Formula: C14H8Cl2O2S2
SMILES: O=C(Sc1ccc(Cl)cc1)C(=O)Sc1ccc(Cl)cc1
Mol. weight [g/mol]: 343.25
CAS: 24455-25-2

Physical Properties

Property code	Value	Unit	Source
gf	57.10	kJ/mol	Joback Method
hf	-55.07	kJ/mol	Joback Method
hfus	39.17	kJ/mol	Joback Method
hvap	88.53	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.931		Crippen Method
mcvol	220.920	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	903.20	K	Joback Method
tc	1188.84	K	Joback Method
tf	553.92	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.97	J/mol×K	903.20	Joback Method
cpg	539.18	J/mol×K	950.81	Joback Method
cpg	546.02	J/mol×K	998.41	Joback Method
cpg	551.58	J/mol×K	1046.02	Joback Method
cpg	555.90	J/mol×K	1093.63	Joback Method
cpg	559.06	J/mol×K	1141.23	Joback Method
cpg	561.12	J/mol×K	1188.84	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=C24455252&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