Phenoxathiin, 2-chloro-

Other names: 2-Chlorophenoxathiin
Inchi: InChI=1S/C12H7ClOS/c13-8-5-6-10-12(7-8)15-11-4-2-1-3-9(11)14-10/h1-7H
InchiKey: QQGJRVZIBGEUGZ-UHFFFAOYSA-N
Formula: C12H7ClOS
SMILES: Clc1ccc2c(c1)Sc1ccccc1O2
Mol. weight [g/mol]: 234.70
CAS: 10230-34-9

Physical Properties

Property code	Value	Unit	Source
gf	268.46	kJ/mol	Joback Method
hf	144.46	kJ/mol	Joback Method
hfus	28.75	kJ/mol	Joback Method
hvap	63.60	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	4.597		Crippen Method
mcvol	156.020	ml/mol	McGowan Method
pc	3598.56	kPa	Joback Method
tb	661.61	K	Joback Method
tc	935.83	K	Joback Method
tf	481.04	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.94	J/mol×K	661.61	Joback Method
cpg	362.46	J/mol×K	707.31	Joback Method
cpg	372.91	J/mol×K	753.02	Joback Method
cpg	382.46	J/mol×K	798.72	Joback Method
cpg	391.25	J/mol×K	844.42	Joback Method
cpg	399.45	J/mol×K	890.12	Joback Method
cpg	407.21	J/mol×K	935.83	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10230349&Units=SI

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