

2-(2',4',6'-Trichlorophenoxy)-4-methylthio-aceto-p

Inchi:	InChI=1S/C15H11Cl3O2S/c1-8(19)11-4-3-10(21-2)7-14(11)20-15-12(17)5-9(16)6-13(15)
InchiKey:	RUFFIEBWNLDHNC-UHFFFAOYSA-N
Formula:	C15H11Cl3O2S
SMILES:	CS1ccc(C(C)=O)c(Oc2c(Cl)cc(Cl)cc2Cl)c1
Mol. weight [g/mol]:	361.67
CAS:	116465-23-7

Physical Properties

Property code	Value	Unit	Source
gf	15.50	kJ/mol	Joback Method
hf	-187.37	kJ/mol	Joback Method
hfus	40.25	kJ/mol	Joback Method
hvap	85.97	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	6.364		Crippen Method
mcvol	235.200	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
tb	878.22	K	Joback Method
tc	1139.69	K	Joback Method
tf	570.57	K	Joback Method
vc	0.884	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	575.07	J/molxK	878.22	Joback Method
cpg	585.06	J/molxK	921.80	Joback Method
cpg	593.80	J/molxK	965.38	Joback Method
cpg	601.30	J/molxK	1008.95	Joback Method
cpg	607.58	J/molxK	1052.53	Joback Method
cpg	612.65	J/molxK	1096.11	Joback Method
cpg	616.53	J/molxK	1139.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116465237&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

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