2,3,3-Trichloroacrylic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C9H2Cl6O2/c10-3-1-5(12)6(2-4(3)11)17-9(16)7(13)8(14)15/h1-2H
InchiKey: DAWWNBVHPCMBEQ-UHFFFAOYSA-N
Formula: C9H2Cl6O2
SMILES: O=C(Oc1cc(Cl)c(Cl)cc1Cl)C(Cl)=C(Cl)Cl
Mol. weight [g/mol]: 354.83
CAS: 2224-98-8

Physical Properties

Property code	Value	Unit	Source
gf	-133.96	kJ/mol	Joback Method
hf	-268.57	kJ/mol	Joback Method
hfus	37.49	kJ/mol	Joback Method
hvap	75.47	kJ/mol	Joback Method
log10ws	-6.06		Crippen Method
logp	5.438		Crippen Method
mcvol	190.490	ml/mol	McGowan Method
pc	2741.15	kPa	Joback Method
tb	751.73	K	Joback Method
tc	1008.84	K	Joback Method
tf	473.85	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.72	J/mol×K	751.73	Joback Method
cpg	359.95	J/mol×K	794.58	Joback Method
cpg	365.57	J/mol×K	837.43	Joback Method
cpg	370.62	J/mol×K	880.28	Joback Method
cpg	375.13	J/mol×K	923.14	Joback Method
cpg	379.15	J/mol×K	965.99	Joback Method
cpg	382.72	J/mol×K	1008.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2224988&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