

2,3,3-Trichloroacrylic acid, pentachlorophenyl ester

Inchi:	InChI=1S/C9Cl8O2/c10-1-2(11)4(13)7(5(14)3(1)12)19-9(18)6(15)8(16)17
InchiKey:	YYWRLRGQSRUHAU-UHFFFAOYSA-N
Formula:	C9Cl8O2
SMILES:	O=C(Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl)C(Cl)=C(Cl)Cl
Mol. weight [g/mol]:	423.72
CAS:	3881-57-0

Physical Properties

Property code	Value	Unit	Source
gf	-177.08	kJ/mol	Joback Method
hf	-322.99	kJ/mol	Joback Method
hfus	45.11	kJ/mol	Joback Method
hvap	85.57	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.745		Crippen Method
mcvol	214.970	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
tb	836.55	K	Joback Method
tc	1098.10	K	Joback Method
tf	558.73	K	Joback Method
vc	0.830	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.33	J/molxK	836.55	Joback Method
cpg	382.79	J/molxK	880.14	Joback Method
cpg	386.74	J/molxK	923.73	Joback Method
cpg	390.19	J/molxK	967.32	Joback Method
cpg	393.19	J/molxK	1010.92	Joback Method
cpg	395.75	J/molxK	1054.51	Joback Method
cpg	397.91	J/molxK	1098.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3881570&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
mccvol:	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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