3-Methylbut-2-enoic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C11H8Cl4O2/c1-5(2)3-8(16)17-11-7(13)4-6(12)9(14)10(11)15/h3-4H,1-2H3
InchiKey: KBXBZXPNUPCMKF-UHFFFAOYSA-N
Formula: C11H8Cl4O2
SMILES: CC(C)=CC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 313.99

Physical Properties

Property code	Value	Unit	Source
gf	-94.34	kJ/mol	Joback Method
hf	-280.05	kJ/mol	Joback Method
hfus	35.20	kJ/mol	Joback Method
hvap	71.74	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.172		Crippen Method
mcvol	194.190	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	727.73	K	Joback Method
tc	966.83	K	Joback Method
tf	463.03	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.16	J/mol×K	727.73	Joback Method
cpg	423.67	J/mol×K	767.58	Joback Method
cpg	432.46	J/mol×K	807.43	Joback Method
cpg	440.59	J/mol×K	847.28	Joback Method
cpg	448.05	J/mol×K	887.13	Joback Method
cpg	454.90	J/mol×K	926.98	Joback Method
cpg	461.14	J/mol×K	966.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355133&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume