3-Methylbut-2-enoic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C11H9Cl3O2/c1-6(2)3-11(15)16-10-5-8(13)7(12)4-9(10)14/h3-5H,1-2H3

InchiKey: RIWFJYJVQGPRGX-UHFFFAOYSA-N

Formula: C11H9Cl3O2

SMILES: CC(C)=CC(=O)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 279.55

Physical Properties

Property code	Value	Unit	Source
gf	-72.78	kJ/mol	Joback Method
hf	-252.84	kJ/mol	Joback Method
hfus	31.39	kJ/mol	Joback Method
hvap	66.69	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.518		Crippen Method
mcvol	181.950	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1900.00		NIST Webbook
tb	685.32	K	Joback Method
tc	921.11	K	Joback Method
tf	420.59	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.39	J/mol×K	685.32	Joback Method
cpg	405.95	J/mol×K	724.62	Joback Method
cpg	415.76	J/mol×K	763.92	Joback Method
cpg	424.86	J/mol×K	803.22	Joback Method
cpg	433.26	J/mol×K	842.51	Joback Method
cpg	441.01	J/mol×K	881.81	Joback Method
cpg	448.13	J/mol×K	921.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355132&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

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