3-Methylbut-2-enoic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C11H11ClO2/c1-8(2)7-11(13)14-10-5-3-9(12)4-6-10/h3-7H,1-2H3
InchiKey: CFKIJEHSEFGFHA-UHFFFAOYSA-N
Formula: C11H11ClO2
SMILES: CC(C)=CC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 210.66

Physical Properties

Property code	Value	Unit	Source
gf	-29.66	kJ/mol	Joback Method
hf	-198.42	kJ/mol	Joback Method
hfus	23.77	kJ/mol	Joback Method
hvap	56.60	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.212		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1538.00		NIST Webbook
tb	600.50	K	Joback Method
tc	828.28	K	Joback Method
tf	335.71	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.06	J/mol×K	600.50	Joback Method
cpg	364.94	J/mol×K	638.46	Joback Method
cpg	376.97	J/mol×K	676.43	Joback Method
cpg	388.18	J/mol×K	714.39	Joback Method
cpg	398.61	J/mol×K	752.35	Joback Method
cpg	408.30	J/mol×K	790.32	Joback Method
cpg	417.29	J/mol×K	828.28	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307593&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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