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

Inchi: InChI=1S/C11H10Cl2O2/c1-7(2)5-11(14)15-8-3-4-9(12)10(13)6-8/h3-6H,1-2H3
InchiKey: ZFPKWERGBZSOTQ-UHFFFAOYSA-N
Formula: C11H10Cl2O2
SMILES: CC(C)=CC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 245.10

Physical Properties

Property code	Value	Unit	Source
gf	-51.22	kJ/mol	Joback Method
hf	-225.63	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	61.64	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.865		Crippen Method
mcvol	169.710	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
tb	642.91	K	Joback Method
tc	874.97	K	Joback Method
tf	378.15	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	374.76	J/mol×K	642.91	Joback Method
cpg	386.44	J/mol×K	681.59	Joback Method
cpg	397.33	J/mol×K	720.26	Joback Method
cpg	407.45	J/mol×K	758.94	Joback Method
cpg	416.84	J/mol×K	797.62	Joback Method
cpg	425.54	J/mol×K	836.29	Joback Method
cpg	433.57	J/mol×K	874.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307597&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