Benzeneacetic acid, 4-chloro-, 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C13H15ClO2/c1-10(2)7-8-16-13(15)9-11-3-5-12(14)6-4-11/h3-7H,8-9H2,1-2H3

InchiKey: CGDMGJNRMZYCOK-UHFFFAOYSA-N

Formula: C13H15ClO2

SMILES: CC(C)=CCOC(=O)Cc1ccc(Cl)cc1

Mol. weight [g/mol]: 238.71

Physical Properties

Property code	Value	Unit	Source
gf	-12.82	kJ/mol	Joback Method
hf	-239.70	kJ/mol	Joback Method
hfus	28.95	kJ/mol	Joback Method
hvap	61.05	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.392		Crippen Method
mcvol	185.650	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook
tb	646.26	K	Joback Method
tc	865.75	K	Joback Method
tf	358.25	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.44	J/mol×K	646.26	Joback Method
cpg	463.69	J/mol×K	682.84	Joback Method
cpg	477.03	J/mol×K	719.42	Joback Method
cpg	489.50	J/mol×K	756.00	Joback Method
cpg	501.13	J/mol×K	792.59	Joback Method
cpg	511.98	J/mol×K	829.17	Joback Method
cpg	522.08	J/mol×K	865.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406997&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