Benzoic acid, 4-chloro, 1-methyl-3-butenyl ester

Inchi: InChI=1S/C12H13ClO2/c1-3-4-9(2)15-12(14)10-5-7-11(13)8-6-10/h3,5-9H,1,4H2,2H3
InchiKey: RRBRGAXTEHCQAZ-UHFFFAOYSA-N
Formula: C12H13ClO2
SMILES: C=CCC(C)OC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 224.68

Physical Properties

Property code	Value	Unit	Source
gf	-7.51	kJ/mol	Joback Method
hf	-206.34	kJ/mol	Joback Method
hfus	22.67	kJ/mol	Joback Method
hvap	57.73	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.461		Crippen Method
mcvol	171.560	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	1519.00		NIST Webbook
rinpol	1534.00		NIST Webbook
ripol	2096.00		NIST Webbook
ripol	2059.00		NIST Webbook
tb	615.58	K	Joback Method
tc	835.06	K	Joback Method
tf	349.26	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.48	J/mol×K	615.58	Joback Method
cpg	414.16	J/mol×K	652.16	Joback Method
cpg	426.97	J/mol×K	688.74	Joback Method
cpg	438.94	J/mol×K	725.32	Joback Method
cpg	450.09	J/mol×K	761.90	Joback Method
cpg	460.46	J/mol×K	798.48	Joback Method

cpg	470.06	J/mol×K	835.06	Joback Method
dvisc	0.0018480	Pa×s	349.26	Joback Method
dvisc	0.0009895	Pa×s	393.65	Joback Method
dvisc	0.0006014	Pa×s	438.03	Joback Method
dvisc	0.0004005	Pa×s	482.42	Joback Method
dvisc	0.0002857	Pa×s	526.81	Joback Method
dvisc	0.0002148	Pa×s	571.19	Joback Method
dvisc	0.0001682	Pa×s	615.58	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=R31131&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume