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

Inchi: InChI=1S/C12H13ClO2/c1-3-5-9(2)15-12(14)10-6-4-7-11(13)8-10/h3-4,6-9H,1,5H2,2H3

InchiKey: CELDXIWRLNPHGJ-UHFFFAOYSA-N

Formula: C12H13ClO2

SMILES: C=CCC(C)OC(=O)c1cccc(Cl)c1

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	1526.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1524.00		NIST Webbook
rinpol	1514.00		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1533.00		NIST Webbook
rinpol	1517.00		NIST Webbook
ripol	2093.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2091.00		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2091.00		NIST Webbook
ripol	2057.00		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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R31056&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
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