Benzoic acid, 2-chloro, 3-butenyl ester

Inchi: InChI=1S/C11H11ClO2/c1-2-3-8-14-11(13)9-6-4-5-7-10(9)12/h2,4-7H,1,3,8H2
InchiKey: GSTHBFGBLMWSHY-UHFFFAOYSA-N
Formula: C11H11ClO2
SMILES: C=CCCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 210.66

Physical Properties

Property code	Value	Unit	Source
gf	-13.49	kJ/mol	Joback Method
hf	-180.42	kJ/mol	Joback Method
hfus	23.60	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.073		Crippen Method
mcvol	157.470	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
rinpol	1494.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1498.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1505.00		NIST Webbook
ripol	2183.00		NIST Webbook
ripol	2196.00		NIST Webbook
ripol	2167.00		NIST Webbook
ripol	2167.00		NIST Webbook
ripol	2186.00		NIST Webbook
ripol	2209.00		NIST Webbook
ripol	2217.00		NIST Webbook
tb	593.14	K	Joback Method
tc	811.98	K	Joback Method
tf	352.99	K	Joback Method
vc	0.598	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	352.26	J/mol×K	593.14	Joback Method
cpg	364.87	J/mol×K	629.61	Joback Method
cpg	376.70	J/mol×K	666.09	Joback Method
cpg	387.76	J/mol×K	702.56	Joback Method
cpg	398.08	J/mol×K	739.03	Joback Method
cpg	407.69	J/mol×K	775.50	Joback Method
cpg	416.61	J/mol×K	811.98	Joback Method
dvisc	0.0015687	Pa×s	352.99	Joback Method
dvisc	0.0009325	Pa×s	393.01	Joback Method
dvisc	0.0006103	Pa×s	433.04	Joback Method
dvisc	0.0004291	Pa×s	473.06	Joback Method
dvisc	0.0003187	Pa×s	513.09	Joback Method
dvisc	0.0002472	Pa×s	553.12	Joback Method
dvisc	0.0001984	Pa×s	593.14	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R31006&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