Butanoic acid, 4-chloro, 3-butenyl ester

Inchi: InChI=1S/C8H13ClO2/c1-2-3-7-11-8(10)5-4-6-9/h2H,1,3-7H2
InchiKey: BRFXAUYDTUPHNQ-UHFFFAOYSA-N
Formula: C8H13ClO2
SMILES: C=CCCOC(=O)CCCCl
Mol. weight [g/mol]: 176.64

Physical Properties

Property code	Value	Unit	Source
gf	-141.53	kJ/mol	Joback Method
hf	-343.56	kJ/mol	Joback Method
hfus	22.18	kJ/mol	Joback Method
hvap	46.27	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	2.125		Crippen Method
mcvol	138.960	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	1187.00		NIST Webbook
rinpol	1200.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1187.00		NIST Webbook
rinpol	1171.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1749.00		NIST Webbook
ripol	1765.00		NIST Webbook
tb	492.84	K	Joback Method
tc	677.25	K	Joback Method
tf	280.24	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.99	J/mol×K	492.84	Joback Method
cpg	301.21	J/mol×K	523.58	Joback Method

cpg	311.96	J/mol×K	554.31	Joback Method
cpg	322.24	J/mol×K	585.05	Joback Method
cpg	332.06	J/mol×K	615.78	Joback Method
cpg	341.43	J/mol×K	646.52	Joback Method
cpg	350.35	J/mol×K	677.25	Joback Method
dvisc	0.0028366	Pa×s	280.24	Joback Method
dvisc	0.0015319	Pa×s	315.67	Joback Method
dvisc	0.0009369	Pa×s	351.11	Joback Method
dvisc	0.0006270	Pa×s	386.54	Joback Method
dvisc	0.0004489	Pa×s	421.97	Joback Method
dvisc	0.0003385	Pa×s	457.41	Joback Method
dvisc	0.0002658	Pa×s	492.84	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R28956&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