Butanoic acid, 3-chloro, 4-pentenyl ester

Inchi: InChI=1S/C9H15ClO2/c1-3-4-5-6-12-9(11)7-8(2)10/h3,8H,1,4-7H2,2H3
InchiKey: IOWBXHKVYVQZBG-UHFFFAOYSA-N
Formula: C9H15ClO2
SMILES: C=CCCCOC(=O)CC(C)Cl
Mol. weight [g/mol]: 190.67

Physical Properties

Property code	Value	Unit	Source
gf	-135.55	kJ/mol	Joback Method
hf	-369.48	kJ/mol	Joback Method
hfus	21.25	kJ/mol	Joback Method
hvap	48.11	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.513		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
rinpol	1220.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1205.00		NIST Webbook
rinpol	1232.00		NIST Webbook
ripol	1748.00		NIST Webbook
ripol	1781.00		NIST Webbook
ripol	1732.00		NIST Webbook
tb	515.28	K	Joback Method
tc	701.54	K	Joback Method
tf	276.51	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.91	J/mol×K	515.28	Joback Method
cpg	391.04	J/mol×K	670.50	Joback Method
cpg	380.68	J/mol×K	639.46	Joback Method

cpg	369.80	J/mol×K	608.41	Joback Method
cpg	358.38	J/mol×K	577.37	Joback Method
cpg	346.42	J/mol×K	546.32	Joback Method
cpg	400.89	J/mol×K	701.54	Joback Method
dvisc	0.0002319	Pa×s	515.28	Joback Method
dvisc	0.0003042	Pa×s	475.48	Joback Method
dvisc	0.0004192	Pa×s	435.69	Joback Method
dvisc	0.0006163	Pa×s	395.89	Joback Method
dvisc	0.0009875	Pa×s	356.10	Joback Method
dvisc	0.0017815	Pa×s	316.31	Joback Method
dvisc	0.0038090	Pa×s	276.51	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R28821&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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