Butanoic acid, 4-chloro, (E)-3-hexenyl ester

Inchi: InChI=1S/C10H17ClO2/c1-2-3-4-5-9-13-10(12)7-6-8-11/h3-4H,2,5-9H2,1H3/b4-3+
InchiKey: JAWDGGOEFQDOMJ-ONEGZZNKSA-N
Formula: C10H17ClO2
SMILES: CCC=CCCOC(=O)CCCCl
Mol. weight [g/mol]: 204.69

Physical Properties

Property code	Value	Unit	Source
gf	-132.31	kJ/mol	Joback Method
hf	-393.05	kJ/mol	Joback Method
hfus	28.84	kJ/mol	Joback Method
hvap	51.35	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.905		Crippen Method
mcvol	167.140	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	1402.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1377.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1385.00		NIST Webbook
ripol	1960.00		NIST Webbook
ripol	1924.00		NIST Webbook
ripol	1935.00		NIST Webbook
ripol	1875.00		NIST Webbook
ripol	1875.00		NIST Webbook
tb	546.08	K	Joback Method
tc	730.87	K	Joback Method
tf	299.46	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	379.88	J/mol×K	546.08	Joback Method
cpg	440.01	J/mol×K	700.07	Joback Method
cpg	429.13	J/mol×K	669.27	Joback Method
cpg	417.70	J/mol×K	638.48	Joback Method
cpg	405.69	J/mol×K	607.68	Joback Method
cpg	393.09	J/mol×K	576.88	Joback Method
cpg	450.34	J/mol×K	730.87	Joback Method
dvisc	0.0001859	Pa×s	546.08	Joback Method
dvisc	0.0002420	Pa×s	504.98	Joback Method
dvisc	0.0003300	Pa×s	463.87	Joback Method
dvisc	0.0004780	Pa×s	422.77	Joback Method
dvisc	0.0007500	Pa×s	381.67	Joback Method
dvisc	0.0013117	Pa×s	340.56	Joback Method
dvisc	0.0026747	Pa×s	299.46	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=R28988&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

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