Butanoic acid, 2-chloro, (E)-3-hexenyl ester

Inchi: InChI=1S/C10H17ClO2/c1-3-5-6-7-8-13-10(12)9(11)4-2/h5-6,9H,3-4,7-8H2,1-2H3/b6-5+
InchiKey: WKCOAKPPMVZACK-AATRIKPKSA-N
Formula: C10H17ClO2
SMILES: CCC=CCCOC(=O)C(Cl)CC
Mol. weight [g/mol]: 204.69

Physical Properties

Property code	Value	Unit	Source
gf	-134.75	kJ/mol	Joback Method
hf	-398.33	kJ/mol	Joback Method
hfus	25.32	kJ/mol	Joback Method
hvap	50.97	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.903		Crippen Method
mcvol	167.140	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1320.00		NIST Webbook
rinpol	1305.00		NIST Webbook
ripol	1750.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1797.00		NIST Webbook
tb	545.64	K	Joback Method
tc	734.12	K	Joback Method
tf	284.46	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.20	J/mol×K	545.64	Joback Method

cpg	393.74	J/mol×K	577.05	Joback Method
cpg	406.63	J/mol×K	608.47	Joback Method
cpg	418.89	J/mol×K	639.88	Joback Method
cpg	430.56	J/mol×K	671.29	Joback Method
cpg	441.63	J/mol×K	702.71	Joback Method
cpg	452.15	J/mol×K	734.12	Joback Method
dvisc	0.0036477	Pa×s	284.46	Joback Method
dvisc	0.0015709	Pa×s	327.99	Joback Method
dvisc	0.0008241	Pa×s	371.52	Joback Method
dvisc	0.0004950	Pa×s	415.05	Joback Method
dvisc	0.0003275	Pa×s	458.58	Joback Method
dvisc	0.0002328	Pa×s	502.11	Joback Method
dvisc	0.0001748	Pa×s	545.64	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=R28675&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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