

Butanoic acid, 3-chloro, (Z)-3-hexenyl ester

Inchi:	InChI=1S/C10H17ClO2/c1-3-4-5-6-7-13-10(12)8-9(2)11/h4-5,9H,3,6-8H2,1-2H3/b5-4-
InchiKey:	TZCFURZQKLRBPP-PLNGDYQASA-N
Formula:	C10H17ClO2
SMILES:	CCC=CCCOC(=O)CC(C)Cl
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	1321.00		NIST Webbook
rinpol	1336.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1321.00		NIST Webbook
ripol	1855.00		NIST Webbook
ripol	1827.00		NIST Webbook
ripol	1824.00		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:	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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R28849&Units=SI

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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