

Propanoic acid, 3-chloro, 2-propenyl ester

Inchi:	InChI=1S/C6H9ClO2/c1-2-5-9-6(8)3-4-7/h2H,1,3-5H2
InchiKey:	CTPKUPQTROHREC-UHFFFAOYSA-N
Formula:	C6H9ClO2
SMILES:	C=CCOC(=O)CCCl
Mol. weight [g/mol]:	148.59

Physical Properties

Property code	Value	Unit	Source
gf	-158.37	kJ/mol	Joback Method
hf	-302.28	kJ/mol	Joback Method
hfus	17.00	kJ/mol	Joback Method
hvap	41.82	kJ/mol	Joback Method
log10ws	-1.20		Crippen Method
logp	1.345		Crippen Method
mcvol	110.780	ml/mol	McGowan Method
pc	3291.59	kPa	Joback Method
rinpol	1004.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	997.00		NIST Webbook
ripol	1521.00		NIST Webbook
ripol	1516.00		NIST Webbook
ripol	1528.00		NIST Webbook
tb	447.08	K	Joback Method
tc	635.32	K	Joback Method
tf	257.70	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.87	J/mol×K	447.08	Joback Method
cpg	249.84	J/mol×K	603.95	Joback Method

cpg	242.35	J/mol×K	572.57	Joback Method
cpg	234.52	J/mol×K	541.20	Joback Method
cpg	226.33	J/mol×K	509.83	Joback Method
cpg	217.78	J/mol×K	478.45	Joback Method
cpg	256.98	J/mol×K	635.32	Joback Method
dvisc	0.0003006	Pa×s	447.08	Joback Method
dvisc	0.0003781	Pa×s	415.52	Joback Method
dvisc	0.0004939	Pa×s	383.95	Joback Method
dvisc	0.0006767	Pa×s	352.39	Joback Method
dvisc	0.0009864	Pa×s	320.83	Joback Method
dvisc	0.0015611	Pa×s	289.26	Joback Method
dvisc	0.0027648	Pa×s	257.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R113845&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

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