Butanoic acid, 4-chloro, 2-propenyl ester

Inchi: InChI=1S/C7H11ClO2/c1-2-6-10-7(9)4-3-5-8/h2H,1,3-6H2
InchiKey: NSCJTNOFIYBWFN-UHFFFAOYSA-N
Formula: C7H11ClO2
SMILES: C=CCOC(=O)CCCCl
Mol. weight [g/mol]: 162.61

Physical Properties

Property code	Value	Unit	Source
gf	-149.95	kJ/mol	Joback Method
hf	-322.92	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	44.05	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.735		Crippen Method
mcvol	124.870	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
rinpol	1097.00		NIST Webbook
rinpol	1077.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1105.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1692.00		NIST Webbook
tb	469.96	K	Joback Method
tc	656.31	K	Joback Method
tf	268.97	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.36	J/mol×K	469.96	Joback Method
cpg	258.49	J/mol×K	501.02	Joback Method
cpg	268.20	J/mol×K	532.08	Joback Method
cpg	277.49	J/mol×K	563.14	Joback Method

cpg	286.38	J/mol×K	594.19	Joback Method
cpg	294.86	J/mol×K	625.25	Joback Method
cpg	302.94	J/mol×K	656.31	Joback Method
dvisc	0.0028258	Pa×s	268.97	Joback Method
dvisc	0.0015592	Pa×s	302.47	Joback Method
dvisc	0.0009687	Pa×s	335.97	Joback Method
dvisc	0.0006561	Pa×s	369.47	Joback Method
dvisc	0.0004741	Pa×s	402.96	Joback Method
dvisc	0.0003601	Pa×s	436.46	Joback Method
dvisc	0.0002844	Pa×s	469.96	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=R28938&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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