3,3-Dimethylacryloyl chloride

Other names:	3,3-Dimethylacrylyl chloride
	2-Butenoyl chloride, 3-methyl-
	3-methyl-2-butenoyl chloride
Inchi:	InChI=1S/C5H7ClO/c1-4(2)3-5(6)7/h3H,1-2H3
InchiKey:	BDUBTLFQHNYXPC-UHFFFAOYSA-N
Formula:	C5H7ClO
SMILES:	CC(C)=CC(=O)Cl
Mol. weight [g/mol]:	118.56
CAS:	3350-78-5

Physical Properties

Property code	Value	Unit	Source
gf	-77.96	kJ/mol	Joback Method
hf	-167.42	kJ/mol	Joback Method
hfus	13.39	kJ/mol	Joback Method
hvap	37.89	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.718		Crippen Method
mcvol	90.820	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	419.20	K	NIST Webbook
tc	609.30	K	Joback Method
tf	206.92	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.53	J/mol×K	409.14	Joback Method
cpg	158.68	J/mol×K	442.50	Joback Method
cpg	166.38	J/mol×K	475.86	Joback Method
cpg	173.64	J/mol×K	509.22	Joback Method
cpg	180.47	J/mol×K	542.58	Joback Method
cpg	186.92	J/mol×K	575.94	Joback Method

cpg	192.99	J/mol×K	609.30	Joback Method

Sources

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=C3350785&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume