3-METHYL-2-BUTENOYL 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

Physical Properties

Property code	Value	Unit	Source
af	0.3341		Cheméo Relay (1.0)
gf	-77.96	kJ/mol	Joback Method
hf	-218.86	kJ/mol	Cheméo Relay (1.0)
hfus	13.39	kJ/mol	Joback Method
hvap	38.01	kJ/mol	Cheméo Relay (1.0)
ie	9.63	eV	Cheméo Relay (1.0)
logp	1.718		Crippen Method
mcvol	90.820	ml/mol	McGowan Method
pc	3834.03	kPa	Joback Method
tb	411.30	K	Cheméo Relay (1.0)
tc	594.43	K	Cheméo Relay (1.0)
tf	204.15	K	Cheméo Relay (1.0)
vc	0.323	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3350785&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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