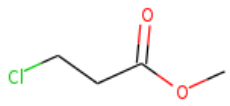
Propanoic acid, 3-chloro-, methyl ester

Other names: Methyl 3-chloropropionate; Propionic acid, 3-chloro-, methyl ester; USAF do-7.
InChI: InChI=1S/C4H7ClO2/c1-7-4(6)2-3-5/h2-3H2,1H3
InChI Key: GZGJIACHBCQSPC-UHFFFAOYSA-N
Formula: C4H7ClO2
SMILES: COC(=O)CCCl
Molecular Weight: 122.55
CAS: 6001-87-2



Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{liquid}$	-2098.00	kJ/mol	NIST Webbook
$\Delta_f G°$	-263.05	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-386.43	kJ/mol	Joback Method
$\Delta_{fus} H°$	13.10	kJ/mol	Joback Method
$\Delta_{vap} H°$	38.04	kJ/mol	Joback Method
$log P_{oct/wat}$	0.79		Crippen Method
P_c	3940.66	kPa	Joback Method
T_{boil}	429.20	K	NIST Webbook
T_c	592.13	K	Joback Method
T_{fus}	236.92	K	Joback Method
V_c	0.33	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	151.10	J/mol×K	404.64	Joback Method
η	0.00	Pa×s	404.64	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C4H7ClO2/c1-7-4(6)2-3-5/h2-3H2,1H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

Δ_c**H°**$_{liquid}$: Standard liquid enthalpy of combustion (kJ/mol).
C$_{p,gas}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
Δ_f**G°**: Standard Gibbs free energy of formation (kJ/mol).
Δ_f**H°**$_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
Δ_{fus}**H°**: Enthalpy of fusion at standard conditions (kJ/mol).
Δ_{vap}**H°**: Enthalpy of vaporization at standard conditions (kJ/mol).
***log*P**$_{oct/wat}$: Octanol/Water partition coefficient .
P$_c$: Critical Pressure (kPa).
T$_{boil}$: Normal Boiling Point Temperature (K).
T$_c$: Critical Temperature (K).
T$_{fus}$: Normal melting (fusion) point (K).
V$_c$: Critical Volume (m^3/kg-mol).