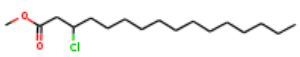
3-Chlorohexadecanoic acid, methyl ester

InChI: InChI=1S/C17H33ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-16(18)15-17(19)20-2/h16H,3-15H2,1-2H3
InChI Key: ZWSOWVGTXJXORW-UHFFFAOYSA-N
Formula: C17H33ClO2
SMILES: CCCCCCCCCCCCCC(Cl)CC(=O)OC
Molecular Weight: 304.90



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-156.03	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-660.03	kJ/mol	Joback Method
$\Delta_{fus} H°$	43.25	kJ/mol	Joback Method
$\Delta_{vap} H°$	66.59	kJ/mol	Joback Method
$logP_{oct/wat}$	5.858		Crippen Method
P_c	1245.97	kPa	Joback Method
T_{boil}	701.64	K	Joback Method
T_c	876.28	K	Joback Method
T_{fus}	368.43	K	Joback Method
V_c	1.054	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	767.83	J/mol×K	701.64	Joback Method
η	0.0000891	Pa×s	701.64	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C17H33ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-16(18)15-17(19)20-2/h16H,3-15H2,1-2H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).