

3-Chlorohexadecanoic acid, methyl ester

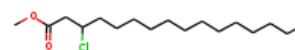
InChI: InChI=1S/C17H33ClO2/c1-3-4-5-6-7-8-9-10-11-12-13-14-16(18)15-17(19)20-2/h16H,3-15H2,1-2H3

InChI Key: ZWSOWVGTXJXORW-UHFFFAOYSA-N

Formula: C17H33ClO2

SMILES: CCCCCCCCCCCCC(Cl)CC(=O)OC

Molecular Weight: 304.90



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-156.03	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-660.03	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	43.25	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	66.59	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	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
$C_{p,\text{gas}}$	767.83	J/mol×K	701.64	Joback Method
η	0.0000891	Paxs	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](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/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/molxK).

η : Dynamic viscosity (Pa \times s).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: 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 (m³/kg-mol).

Latest version available from:

<https://www.chemeo.com/cid/10-234-0/3-Chlorohexadecanoic%20acid%2C%20methyl%20ester>

Generated by Cheméo on Wed, 15 Aug 2018 23:13:53 +0000.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.