

Sebacic acid, 10-chlorodecyl hexyl ester

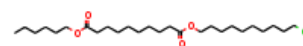
InChI: InChI=1S/C26H49ClO4/c1-2-3-4-18-23-30-25(28)20-15-11-7-8-12-16-21-26(29)31-24-19-14-10-6-5-9-13-17-22-27/h2-24H2,1H3

InChI Key: XXCUKWBJRWIGE-UHFFFAOYSA-N

Formula: C₂₆H₄₉ClO₄

SMILES: CCCCCCOC(=O)CCCCCCCCCC(=O)OCCCCCCCCCCCl

Molecular Weight: 461.12



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-311.73	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1085.31	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	72.87	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	96.17	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	8.13		Crippen Method
P_c	746.92	kPa	Joback Method
T_{boil}	984.29	K	Joback Method
T_c	1216.16	K	Joback Method
T_{fus}	557.02	K	Joback Method
V_c	1.59	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1375.47	J/mol×K	984.29	Joback Method
η	0.00	Paxs	984.29	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C26H49ClO4/c1-2-3-4-18-23-30-25\(28\)20-15-11-7-8-12-16-21-26\(29\)31-24-19-14-10-6-5-9-13-17-22-27/h2-24H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C26H49ClO4/c1-2-3-4-18-23-30-25(28)20-15-11-7-8-12-16-21-26(29)31-24-19-14-10-6-5-9-13-17-22-27/h2-24H2,1H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

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

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: 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.cheméo.com/cid/10-320-4/Sebacic%20acid%2C%2010-chlorodecyl%20hexyl%20ester>

Generated by Cheméo on Tue, 28 Sep 2021 20:05:21 +0000.

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