

Sebacic acid, octyl undecyl ester

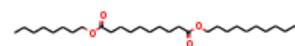
InChI: InChI=1S/C29H56O4/c1-3-5-7-9-11-12-15-19-23-27-33-29(31)25-2
1-17-14-13-16-20-24-28(30)32-26-22-18-10-8-6-4-2/h3-27H2,1-2H3

InChI Key: WPQFVYLUOACTIM-UHFFFAOYSA-N

Formula: C29H56O4

SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCC

Molecular Weight: 468.75



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-274.54	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1131.49	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	76.44	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	98.46	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	9.08		Crippen Method
P_c	654.10	kPa	Joback Method
T_{boil}	1015.50	K	Joback Method
T_c	1268.62	K	Joback Method
T_{fus}	560.91	K	Joback Method
V_c	1.71	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1539.74	J/mol×K	1015.5	Joback Method
η	0.00	Paxs	1015.5	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C29H56O4/c1-3-5-7-9-11-12-15-19-23-27-33-29\(31\)25-21-17-14-13-16-20-24-28\(30\)32-26-22-18-10-8-6-4-2/h3-27H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C29H56O4/c1-3-5-7-9-11-12-15-19-23-27-33-29(31)25-21-17-14-13-16-20-24-28(30)32-26-22-18-10-8-6-4-2/h3-27H2,1-2H3)

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

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).

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