

Sebacic acid, decyl 2-methylpent-3-yl ester

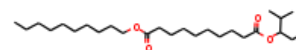
InChI: InChI=1S/C26H50O4/c1-5-7-8-9-10-13-16-19-22-29-25(27)20-17-14-11-12-15-18-21-26(28)30-24(6-2)23(3)4/h23-24H,5-22H2,1-4H3

InChI Key: JVZVAFDIRMIOHL-UHFFFAOYSA-N

Formula: C26H50O4

SMILES: CCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(CC)C(C)C

Molecular Weight: 426.67



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-304.68	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1080.13	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	61.62	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	91.01	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	7.77		Crippen Method
P_c	769.04	kPa	Joback Method
T_{boil}	945.98	K	Joback Method
T_c	1162.69	K	Joback Method
T_{fus}	497.10	K	Joback Method
V_c	1.53	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1345.96	J/mol×K	945.98	Joback Method
η	0.00	Paxs	945.98	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C26H50O4/c1-5-7-8-9-10-13-16-19-22-29-25\(27\)20-17-14-11-12-15-18-21-26\(28\)30-24\(6-2\)23\(3\)4/h23-24H,5-22H2,1-4H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C26H50O4/c1-5-7-8-9-10-13-16-19-22-29-25(27)20-17-14-11-12-15-18-21-26(28)30-24(6-2)23(3)4/h23-24H,5-22H2,1-4H3)

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).

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