

Sebacic acid, 2,4-dimethylpent-3-yl pentadecyl ester

InChI: InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-24-27-35-30(33)25-22-19-16-17-20-23-26-31(34)36-32(28(2)3)29(4)5/h28-29,32H,6-27H2,1-5H3

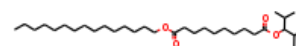
InChI Key: IQDRZKWTALQNie-UHFFFAOYSA-N

Formula: C₃₂H₆₂O₄

SMILES:

CCCCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(C(C)C)C(C)C

Molecular Weight: 510.83



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-256.60	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1209.25	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	73.64	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	103.97	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	9.97		Crippen Method
P_c	573.98	kPa	Joback Method
T_{boil}	1082.82	K	Joback Method
T_c	1370.02	K	Joback Method
T_{fus}	549.72	K	Joback Method
V_c	1.86	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1737.08	J/mol×K	1082.82	Joback Method
η	0.00	Paxs	1082.82	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-24-27-35-30\(33\)25-22-19-16-17-20-23-26-31\(34\)36-32\(28\(2\)3\)29\(4\)5/h28-29,32H,6-27H2,1-5H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C32H62O4/c1-6-7-8-9-10-11-12-13-14-15-18-21-24-27-35-30(33)25-22-19-16-17-20-23-26-31(34)36-32(28(2)3)29(4)5/h28-29,32H,6-27H2,1-5H3)

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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