

Pimelic acid, 2-methylpropyl tetradecyl ester

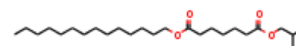
InChI: InChI=1S/C25H48O4/c1-4-5-6-7-8-9-10-11-12-13-14-18-21-28-24(26)19-16-15-17-20-25(27)29-22-23(2)3/h23H,4-22H2,1-3H3

InChI Key: HQUQFOBTLMDXFD-UHFFFAOYSA-N

Formula: C₂₅H₄₈O₄

SMILES: CCCCCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)C

Molecular Weight: 412.65



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-310.66	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-1054.21	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	62.56	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	89.17	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	7.38		Crippen Method
P_c	807.99	kPa	Joback Method
T_{boil}	923.54	K	Joback Method
T_c	1133.47	K	Joback Method
T_{fus}	500.83	K	Joback Method
V_c	1.48	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1281.56	J/mol×K	923.54	Joback Method
η	0.00	Paxs	923.54	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H48O4/c1-4-5-6-7-8-9-10-11-12-13-14-18-21-28-24\(26\)19-16-15-17-20-25\(27\)29-22-23\(2\)3/h23H,4-22H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H48O4/c1-4-5-6-7-8-9-10-11-12-13-14-18-21-28-24(26)19-16-15-17-20-25(27)29-22-23(2)3/h23H,4-22H2,1-3H3)

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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