Adipic acid, 2-methylpent-3-yl pentadecyl ester

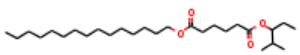
InChI: InChI=1S/C27H52O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-20-23-30-26(28)21-18-19-22-27(29)31-25(6-2)24(3)4/h24-25H,5-23H2,1-4H3

InChI Key: PSSINWQTQMAFQJ-UHFFFAOYSA-N

Formula: C27H52O4

SMILES: CCCCCCCCCCCCCCCOC(=O)CCCCC(=O)OC(CC)C(C)C

Molecular Weight: 440.70



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	-296.26	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-1100.77	kJ/mol	Joback Method
$\Delta_{fus} H°$	64.21	kJ/mol	Joback Method
$\Delta_{vap} H°$	93.23	kJ/mol	Joback Method
$logP_{oct/wat}$	8.16		Crippen Method
P_c	729.67	kPa	Joback Method
T_{boil}	968.86	K	Joback Method
T_c	1194.47	K	Joback Method
T_{fus}	508.37	K	Joback Method
V_c	1.58	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1410.37	J/mol×K	968.86	Joback Method
η	0.00	Pa×s	968.86	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C27H52O4/c1-5-7-8-9-10-11-12-13-14-15-16-17-20-23-30-26(28)21-18-19-22-27(29)31-25(6-2)24(3)4/h24-25H,5-23H2,1-4H3
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$\mathbf{C_{p,gas}}$: Ideal gas heat capacity (J/mol×K).
η: Dynamic viscosity (Pa×s).
$\Delta_f\mathbf{G°}$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f\mathbf{H°_{gas}}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus}\mathbf{H°}$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap}\mathbf{H°}$: Enthalpy of vaporization at standard conditions (kJ/mol).
$\boldsymbol{log}\mathbf{P_{oct/wat}}$: Octanol/Water partition coefficient .
$\mathbf{P_c}$: Critical Pressure (kPa).
$\mathbf{T_{boil}}$: Normal Boiling Point Temperature (K).
$\mathbf{T_c}$: Critical Temperature (K).
$\mathbf{T_{fus}}$: Normal melting (fusion) point (K).
$\mathbf{V_c}$: Critical Volume (m^3/kg-mol).