

Sebacic acid, geranyl propyl ester

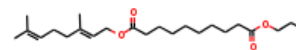
InChI: InChI=1S/C23H40O4/c1-5-18-26-22(24)15-10-8-6-7-9-11-16-23(25)27-19-17-21(4)14-12-13-20(2)3/h13,17H,5-12,14-16,18-19H2,1-4H3/b21-17+

InChI Key: NHDOBNIBFGIIE-HEHNFIMWSA-N

Formula: C23H40O4

SMILES: CCCOC(=O)CCCCCCCCC(=O)OCC=C(C)CCC=C(C)C

Molecular Weight: 380.56



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-181.72	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-792.79	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	58.68	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	85.18	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	6.296		Crippen Method
P_c	964.47	kPa	Joback Method
T_{boil}	886.30	K	Joback Method
T_c	1085.70	K	Joback Method
T_{fus}	455.21	K	Joback Method
V_c	1.333	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	1100.28	J/mol×K	886.3	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H40O4/c1-5-18-26-22\(24\)15-10-8-6-7-9-11-16-23\(25\)27-19-17-21\(4\)14-12-13-20\(2\)3/h13,17H,5-12,14-16,18-19H2,1-4H3/b21-17+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C23H40O4/c1-5-18-26-22(24)15-10-8-6-7-9-11-16-23(25)27-19-17-21(4)14-12-13-20(2)3/h13,17H,5-12,14-16,18-19H2,1-4H3/b21-17+)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p, gas}$: Ideal gas heat capacity (J/mol×K).

$\Delta_f G^\circ$: 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).

$\log P_{oct/wat}$: 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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