(Z,E)-Farnesyl caprate

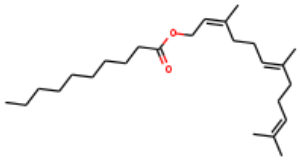
InChI: InChI=1S/C25H44O2/c1-6-7-8-9-10-11-12-19-25(26)27-21-20-24(5)18-14-17-23(4)16-13-15-22(2)3/h15,17,20H,6-14,16,18-19,21H2,1-5H3/b23-17+,24-20-

InChI Key: ZSPZCKNQANJUIH-HTQNKFGOSA-N

Formula: C25H44O2

SMILES: CCCCCCCCCC(=O)OCC=C(C)CCC=C(C)CCC=C(C)C

Molecular Weight: 376.62



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	140.71	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-481.84	kJ/mol	Joback Method
$\Delta_{fus} H°$	59.97	kJ/mol	Joback Method
$\Delta_{vap} H°$	80.51	kJ/mol	Joback Method
$logP_{oct/wat}$	8.09		Crippen Method
P_c	864.54	kPa	Joback Method
T_{boil}	859.81	K	Joback Method
T_c	1054.48	K	Joback Method
T_{fus}	386.55	K	Joback Method
V_c	1.40	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1142.06	J/mol×K	859.81	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C25H44O2/c1-6-7-8-9-10-11-12-19-25(26)27-21-20-24(5)18-14-17-23(4)16-13-15-22(2)3/h15,17,20H,6-14,16,18-19,21H2,1-5H3/b23-17+,24-20-

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).
$\Delta_f G°$: Standard Gibbs free energy of formation (kJ/mol).
$\Delta_f H°_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).
$\Delta_{fus} H°$: Enthalpy of fusion at standard conditions (kJ/mol).
$\Delta_{vap} H°$: 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 (m^3/kg-mol).