

(Z,E)-Farnesyl caprate

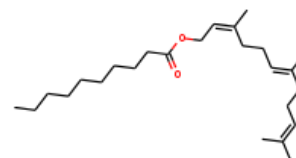
InChI: InChI=1S/C25H44O2/c1-6-7-8-9-10-11-12-19-25(26)27-21-20-24(5)18-14-17-23(4)16-13-15-22(2)3/h15,17,20H,6-14,16,18-19,21H2,1-5H3/b23-17+,24-20-

InChI Key: ZSPZCKNQANJUIH-HTQNKFGOSA-N

Formula: C₂₅H₄₄O₂

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

Molecular Weight: 376.62



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	140.71	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-481.84	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	59.97	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	80.51	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	8.090		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	1.403	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	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-](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/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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