

trans,trans-Farnesoic acid

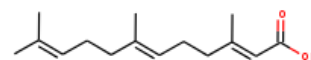
InChI: InChI=1S/C15H24O2/c1-12(2)7-5-8-13(3)9-6-10-14(4)11-15(16)17/h7,9,11H,5-6,8,10H2,1-4H3,(H,16,17)/b13-9+,14-11+

InChI Key: WJHFZYAELPOJIV-IJFRVEDASA-N

Formula: C15H24O2

SMILES: CC(C)=CCCC(C)=CCCC(C)=CC(=O)O

Molecular Weight: 236.35



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	24.69	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-295.45	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	36.97	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	72.52	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	4.49		Crippen Method
P_c	1838.84	kPa	Joback Method
T_{boil}	700.77	K	Joback Method
T_c	887.37	K	Joback Method
T_{fus}	312.44	K	Joback Method
V_c	0.84	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	594.65	J/mol×K	700.77	Joback Method

Sources

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

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H24O2/c1-12\(2\)7-5-8-13\(3\)9-6-10-14\(4\)11-15\(16\)17/h7,9,11H,5-6,8,10H2,1-4H3,\(H,16,17\)/b13-9+,14-11+](http://webbook.nist.gov/cgi/inchi/InChI=1S/C15H24O2/c1-12(2)7-5-8-13(3)9-6-10-14(4)11-15(16)17/h7,9,11H,5-6,8,10H2,1-4H3,(H,16,17)/b13-9+,14-11+)

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

Legend

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

$\Delta_f G^\circ$: 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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