d,«alpha»-Tocopherol

Other names: Tocol, 5,7,8-trimethyl; Vitamin E.

InChI: InChI=1S/C29H50O2/c1-20(2)12-9-13-21(3)14-10-15-22(4)16-11-18-29(8)19-17-26-25(7)27(30)23(5)24(6)28(26)31-29/h20-22,30H,9-19H2,1-8H3/t21-,22-,29-/m0/s1

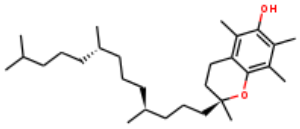
InChI Key: GVJHHUAWPYXKBD-SYZUXVNWSA-N

Formula: C29H50O2

SMILES: Cc1c(C)c2c(c(C)c1O)CCC(C)(CCCC(C)CCCC(C)CCCC(C)C)O2

Molecular Weight: 430.71

CAS: 1406-18-4



Physical Properties

Property	Value	Unit	Source
$\Delta_f G°$	62.29	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-694.51	kJ/mol	Joback Method
$\Delta_{fus} H°$	56.28	kJ/mol	Joback Method
$\Delta_{vap} H°$	100.37	kJ/mol	Joback Method
$logP_{oct/wat}$	8.84		Crippen Method
P_c	882.09	kPa	Joback Method
T_{boil}	1027.02	K	Joback Method
T_c	1257.43	K	Joback Method
T_{fus}	624.70	K	Joback Method
V_c	1.47	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	1437.29	J/mol×K	1027.02	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C29H50O2/c1-20(2)12-9-13-21(3)14-10-15-22(4)16-11-18-29(8)19-17-26-25(7)27(30)23(5)24(6)28(26)31-29/h20-22,30H,9-19H2,1-8H3/t21-,22-,29-/m0/s1

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).