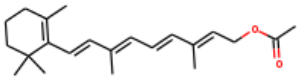
Retinol, acetate



Other names: 3,7-Dimethyl-9-(2,6,6,-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraen-1-ol acetate, (all trans)-; Crystalets; Davitan A 650; Myvak; Myvax; NSC 122045; Retinol, acetate, all-trans-; Retinyl acetate; Ro 1-5275; Vitamin A acetate; Vitamin A alcohol acetate; Vitamin A1 acetate; all-trans-Retinol acetate; all-trans-Retinyl acetate; all-trans-Vitamin A acetate; trans-Retinol acetate; trans-Retinyl acetate; trans-Vitamin A acetate.

InChI: InChI=1S/C22H32O2/c1-17(9-7-10-18(2)14-16-24-20(4)23)12-13-21-19(3)11-8-15-22(21,5)6/h7,9-10,12-14H,8,11,15-16H2,1-6H3/b10-7+,13-12+,17-9+,18-14+

InChI Key: QGNJRVVDBSJHIZ-QHLGVNSISA-N

Formula: C22H32O2

SMILES: CC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C

Molecular Weight: 328.49

CAS: 127-47-9

Physical Properties

Property	Value	Unit	Source
$\Delta_c H°_{solid}$	-11517.70 ± 6.00	kJ/mol	NIST Webbook
$\Delta_f G°$	233.88	kJ/mol	Joback Method
$\Delta_f H°_{gas}$	-188.51	kJ/mol	Joback Method
$\Delta_f H°_{solid}$	-1713.00 ± 6.00	kJ/mol	NIST Webbook
$\Delta_{fus} H°$	39.69	kJ/mol	Joback Method
$\Delta_{vap} H°$	74.61	kJ/mol	Joback Method
$logP_{oct/wat}$	6.081		Crippen Method
P_c	1266.45	kPa	Joback Method
T_{boil}	824.36	K	Joback Method
T_c	1042.16	K	Joback Method
T_{fus}	418.70	K	Joback Method
V_c	1.131	m^3/kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,gas}$	896.69	J/mol×K	824.36	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/inchi/InChI=1S/C22H32O2/c1-17(9-7-10-18(2)14-16-24-20(4)23)12-13-21-19(3)11-8-15-22(21,5)6/h7,9-10,12-14H,8,11,15-16H2,1-6H3/b10-7+,13-12+,17-9+,18-14+

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

Legend

$\Delta_c H°_{solid}$: Standard solid enthalpy of combustion (kJ/mol).
$C_{p,gas}$: 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).
$\Delta_f H°_{solid}$: Solid phase 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).
$logP_{oct/wat}$: 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).