Retinol, acetate

Other names:	Retinol, acetate, all-trans- all-trans-Retinol acetate all-trans-Retinyl acetate all-trans-Vitamin A acetate trans-Retinyl acetate Myvak Myvax Retinyl acetate Vitamin A acetate Vitamin A1 acetate trans-Vitamin A acetate Crystalets Davitan A 650 Vitamin A alcohol acetate 3,7-Dimethyl-9-(2,6,6,-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraen-1-ol acetate, (all trans)- NSC 122045 Ro 1-5275 trans-Retinol 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
InchiKey:	QGNJRVVDBSJHIZ-QHLGVNSISA-N
Formula:	C22H32O2
SMILES:	CC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]:	328.49
CAS:	127-47-9

Physical Properties

Property code	Value	Unit	Source
chs	-11517.70 ± 6.00	kJ/mol	NIST Webbook
gf	233.88	kJ/mol	Joback Method
hf	-188.51	kJ/mol	Joback Method
hfs	-1713.00 ± 6.00	kJ/mol	NIST Webbook
hfus	39.69	kJ/mol	Joback Method
hvap	74.61	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	6.081		Crippen Method
mcvol	295.920	ml/mol	McGowan Method
pc	1266.45	kPa	Joback Method

rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
rinpol	2531.00		NIST Webbook
rinpol	2531.00		NIST Webbook
tb	824.36	K	Joback Method
tc	1042.16	K	Joback Method
tf	418.70	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	896.69	J/mol×K	824.36	Joback Method
cpg	917.44	J/mol×K	860.66	Joback Method
cpg	937.68	J/mol×K	896.96	Joback Method
cpg	957.60	J/mol×K	933.26	Joback Method
cpg	977.38	J/mol×K	969.56	Joback Method
cpg	997.21	J/mol×K	1005.86	Joback Method
cpg	1017.27	J/mol×K	1042.16	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C127479&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume