Vitamin a palmitate

Other names:	Retinol, hexadecanoate
	3,7-Dimethyl-9-(2,6,6,-trimethyl-1-cyclohexen-1-yl)-2,4,6,8-nonatetraen-1-ol palmitate
	Arovit
	Ester found in fish liver oils
	Optovit-A
	retinyl palmitate
Inchi:	InChI=1S/C36H60O2/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-25-35(37)38-30-28-32(3)
InchiKey:	VYGQUTWHTHXGQB-FFHKNEKCSA-N
Formula:	C36H60O2
SMILES:	CCCCCCCCCCCCCCCC(=O)OC/C=C(C)/C=C/C=C(C)/C=C/C1=C(C)CCCC1(C)C
Mol. weight [g/mol]:	524.87

Physical Properties

Property code	Value	Unit	Source
chs	-21292.10 ± 5.90	kJ/mol	NIST Webbook
hfs	-1449.10 ± 5.90	kJ/mol	NIST Webbook
hfus	75.95	kJ/mol	Joback Method
ie	7.34	eV	Cheméo Relay (1.0)
logp	11.543		Crippen Method
mcvol	493.180	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1838.42	J/mol×K	1144.68	Joback Method
cpg	1877.94	J/mol×K	1190.60	Joback Method
cpg	1918.62	J/mol×K	1236.53	Joback Method
cpg	1960.94	J/mol×K	1282.45	Joback Method
cpg	2005.36	J/mol×K	1328.37	Joback Method
cpg	2052.36	J/mol×K	1374.29	Joback Method
cpg	2102.41	J/mol×K	1420.22	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79812&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume