Retinyl dodecanoate

Inchi: InChI=1S/C32H52O2/c1-7-8-9-10-11-12-13-14-15-21-31(33)34-26-24-28(3)19-16-18-27(
InchiKey: ZGISOPBIAXHOTQ-OUGXGHBNSA-N
Formula: C32H52O2
SMILES: CCCCCCCCCCCC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 468.75

Physical Properties

Property code	Value	Unit	Source
gf	318.08	kJ/mol	Joback Method
hf	-394.91	kJ/mol	Joback Method
hfus	65.59	kJ/mol	Joback Method
hvap	96.87	kJ/mol	Joback Method
log10ws	-11.00		Crippen Method
logp	9.982		Crippen Method
mcvol	436.820	ml/mol	McGowan Method
pc	703.59	kPa	Joback Method
rinpol	3577.00		NIST Webbook
tb	1053.16	K	Joback Method
tc	1290.64	K	Joback Method
tf	531.40	K	Joback Method
vc	1.690	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1550.46	J/mol×K	1053.16	Joback Method
cpg	1580.66	J/mol×K	1092.74	Joback Method
cpg	1611.17	J/mol×K	1132.32	Joback Method
cpg	1642.27	J/mol×K	1171.90	Joback Method
cpg	1674.26	J/mol×K	1211.48	Joback Method
cpg	1707.42	J/mol×K	1251.06	Joback Method
cpg	1742.02	J/mol×K	1290.64	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=R55583&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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