Retinyl decanoate

Inchi: InChI=1S/C30H48O2/c1-7-8-9-10-11-12-13-19-29(31)32-24-22-26(3)17-14-16-25(2)20-2
InchiKey: FAPCXJRRCFTZLR-HEYZNTEQSA-N
Formula: C30H48O2
SMILES: CCCCCCCCCC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 440.70

Physical Properties

Property code	Value	Unit	Source
gf	301.24	kJ/mol	Joback Method
hf	-353.63	kJ/mol	Joback Method
hfus	60.41	kJ/mol	Joback Method
hvap	92.42	kJ/mol	Joback Method
log10ws	-10.16		Crippen Method
logp	9.202		Crippen Method
mcvol	408.640	ml/mol	McGowan Method
pc	781.12	kPa	Joback Method
rinpol	3359.00		NIST Webbook
tb	1007.40	K	Joback Method
tc	1233.47	K	Joback Method
tf	508.86	K	Joback Method
vc	1.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1412.07	J/mol×K	1007.40	Joback Method
cpg	1439.23	J/mol×K	1045.08	Joback Method
cpg	1466.46	J/mol×K	1082.76	Joback Method
cpg	1494.00	J/mol×K	1120.44	Joback Method
cpg	1522.09	J/mol×K	1158.12	Joback Method
cpg	1550.96	J/mol×K	1195.79	Joback Method
cpg	1580.85	J/mol×K	1233.47	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=R55579&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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