Retinyl hexanoate

Inchi: InChI=1S/C26H40O2/c1-7-8-9-15-25(27)28-20-18-22(3)13-10-12-21(2)16-17-24-23(4)14
InchiKey: JOHZSPKDCASWAX-BAJOQGENSA-N
Formula: C26H40O2
SMILES: CCCCCC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 384.59

Physical Properties

Property code	Value	Unit	Source
gf	267.56	kJ/mol	Joback Method
hf	-271.07	kJ/mol	Joback Method
hfus	50.05	kJ/mol	Joback Method
hvap	83.51	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	7.641		Crippen Method
mcvol	352.280	ml/mol	McGowan Method
pc	980.23	kPa	Joback Method
rinpol	2970.00		NIST Webbook
tb	915.88	K	Joback Method
tc	1131.30	K	Joback Method
tf	463.78	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1146.53	J/mol×K	915.88	Joback Method
cpg	1169.66	J/mol×K	951.78	Joback Method
cpg	1192.54	J/mol×K	987.69	Joback Method
cpg	1215.36	J/mol×K	1023.59	Joback Method
cpg	1238.30	J/mol×K	1059.49	Joback Method
cpg	1261.57	J/mol×K	1095.40	Joback Method
cpg	1285.35	J/mol×K	1131.30	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=R55597&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

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