Retinyl octanoate

Inchi: InChI=1S/C28H44O2/c1-7-8-9-10-11-17-27(29)30-22-20-24(3)15-12-14-23(2)18-19-26-2
InchiKey: AWGMQQGZWRIUJI-UBMBPVGBSA-N
Formula: C28H44O2
SMILES: CCCCCCCC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 412.65

Physical Properties

Property code	Value	Unit	Source
gf	284.40	kJ/mol	Joback Method
hf	-312.35	kJ/mol	Joback Method
hfus	55.23	kJ/mol	Joback Method
hvap	87.96	kJ/mol	Joback Method
log10ws	-9.33		Crippen Method
logp	8.422		Crippen Method
mcvol	380.460	ml/mol	McGowan Method
pc	872.22	kPa	Joback Method
rinpol	3157.00		NIST Webbook
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tb	961.64	K	Joback Method
tc	1180.54	K	Joback Method
tf	486.32	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.41	J/mol×K	961.64	Joback Method
cpg	1302.27	J/mol×K	998.12	Joback Method
cpg	1327.03	J/mol×K	1034.61	Joback Method
cpg	1351.89	J/mol×K	1071.09	Joback Method
cpg	1377.06	J/mol×K	1107.57	Joback Method
cpg	1402.74	J/mol×K	1144.05	Joback Method
cpg	1429.15	J/mol×K	1180.54	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=R55604&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