Retinyl butanoate

Inchi: InChI=1S/C24H36O2/c1-7-10-23(25)26-18-16-20(3)12-8-11-19(2)14-15-22-21(4)13-9-17
InchiKey: MSHMSHDEYSUBDL-GTHIKWOPSA-N
Formula: C24H36O2
SMILES: CCCC(=O)OCC=C(C)C=CC=C(C)C=CC1=C(C)CCCC1(C)C
Mol. weight [g/mol]: 356.54

Physical Properties

Property code	Value	Unit	Source
gf	250.72	kJ/mol	Joback Method
hf	-229.79	kJ/mol	Joback Method
hfus	44.87	kJ/mol	Joback Method
hvap	79.06	kJ/mol	Joback Method
log10ws	-7.65		Crippen Method
logp	6.861		Crippen Method
mcvol	324.100	ml/mol	McGowan Method
pc	1109.63	kPa	Joback Method
rinpol	2738.00		NIST Webbook
rinpol	2738.00		NIST Webbook
rinpol	2738.00		NIST Webbook
tb	870.12	K	Joback Method
tc	1085.31	K	Joback Method
tf	441.24	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1019.56	J/mol×K	870.12	Joback Method
cpg	1041.37	J/mol×K	905.98	Joback Method
cpg	1062.79	J/mol×K	941.85	Joback Method
cpg	1084.01	J/mol×K	977.71	Joback Method
cpg	1105.22	J/mol×K	1013.58	Joback Method
cpg	1126.60	J/mol×K	1049.44	Joback Method
cpg	1148.33	J/mol×K	1085.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R55565&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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