Acetoxy-copalic acid methyl ester

Inchi: InChI=1S/C23H36O4/c1-15(14-21(25)26-7)8-10-18-16(2)9-11-19-22(4,5)20(27-17(3)24)1
InchiKey: LODVZNAZFNRTCG-XDARRNPMSA-N
Formula: C23H36O4
SMILES: C=C1CCC2C(C)(C)C(OC(C)=O)CCC2(C)C1CCC(C)=CC(=O)OC
Mol. weight [g/mol]: 376.53

Physical Properties

Property code	Value	Unit	Source
gf	-161.32	kJ/mol	Joback Method
hf	-725.56	kJ/mol	Joback Method
hfus	37.12	kJ/mol	Joback Method
hvap	82.59	kJ/mol	Joback Method
log10ws	-5.82		Crippen Method
logp	5.226		Crippen Method
mcvol	319.490	ml/mol	McGowan Method
pc	1183.34	kPa	Joback Method
rinpol	2634.00		NIST Webbook
rinpol	2634.00		NIST Webbook
tb	898.45	K	Joback Method
tc	1118.15	K	Joback Method
tf	544.81	K	Joback Method
vc	1.212	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.67	J/mol×K	898.45	Joback Method
cpg	1115.47	J/mol×K	935.07	Joback Method
cpg	1140.20	J/mol×K	971.68	Joback Method
cpg	1165.09	J/mol×K	1008.30	Joback Method
cpg	1190.35	J/mol×K	1044.92	Joback Method
cpg	1216.20	J/mol×K	1081.54	Joback Method
cpg	1242.86	J/mol×K	1118.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R519372&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