trans-Sabinyl acetate

Inchi: InChI=1S/C12H18O2/c1-7(2)12-5-10(12)8(3)11(6-12)14-9(4)13/h7,10-11H,3,5-6H2,1-2,4
InchiKey: PBWRFXQNNGSAQG-GLXQMMQGSA-N
Formula: C12H18O2
SMILES: C=C1C(OC(C)=O)CC2(C(C)C)CC12
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
hfus	15.98	kJ/mol	Joback Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
rinpol	1275.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1278.00		NIST Webbook
ripol	1650.00		NIST Webbook
ripol	1637.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	417.14	J/mol×K	558.02	Joback Method
cpg	433.79	J/mol×K	592.44	Joback Method
cpg	449.43	J/mol×K	626.85	Joback Method
cpg	464.18	J/mol×K	661.27	Joback Method
cpg	478.16	J/mol×K	695.68	Joback Method
cpg	491.51	J/mol×K	730.10	Joback Method
cpg	504.33	J/mol×K	764.52	Joback Method

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R600532&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices