trans-Sabinyl acetate

Other names: (E)-Sabinyl acetate
Sabinyl acetate, trans
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-SAIIYOCFSA-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	1281.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1290.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1272.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1271.00		NIST Webbook

rinpol	1291.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1298.00	NIST Webbook
rinpol	1296.00	NIST Webbook
rinpol	1275.00	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1277.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1277.00	NIST Webbook
rinpol	1274.00	NIST Webbook
rinpol	1273.00	NIST Webbook
rinpol	1291.00	NIST Webbook
rinpol	1290.00	NIST Webbook
ripol	1643.00	NIST Webbook
ripol	1651.00	NIST Webbook
ripol	1657.00	NIST Webbook
ripol	1622.00	NIST Webbook
ripol	1609.00	NIST Webbook
ripol	1667.00	NIST Webbook
ripol	1664.00	NIST Webbook
ripol	1643.00	NIST Webbook
ripol	1622.00	NIST Webbook
ripol	1664.00	NIST Webbook
ripol	1657.00	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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R269988&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

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