Sabinyl, 2-methylbutanoate

Inchi: InChI=1S/C15H24O2/c1-6-10(4)14(16)17-13-8-15(9(2)3)7-12(15)11(13)5/h9-10,12-13H,5
InchiKey: HXJZQZHCRQMSRY-UHFFFAOYSA-N
Formula: C15H24O2
SMILES: C=C1C(OC(=O)C(C)CC)CC2(C(C)C)CC12
Mol. weight [g/mol]: 236.35

Physical Properties

Property code	Value	Unit	Source
gf	-2.00	kJ/mol	Joback Method
hf	-383.55	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	55.89	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	3.567		Crippen Method
mcvol	203.630	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	1501.10		NIST Webbook
rinpol	1501.10		NIST Webbook
tb	626.22	K	Joback Method
tc	827.69	K	Joback Method
tf	370.19	K	Joback Method
vc	0.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.31	J/mol×K	626.22	Joback Method
cpg	588.78	J/mol×K	659.80	Joback Method
cpg	606.29	J/mol×K	693.38	Joback Method
cpg	622.97	J/mol×K	726.96	Joback Method
cpg	638.96	J/mol×K	760.54	Joback Method
cpg	654.35	J/mol×K	794.11	Joback Method
cpg	669.29	J/mol×K	827.69	Joback Method

Sources

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=U413834&Units=SI
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
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