Sabinyl isobutanoate

Inchi: InChI=1S/C14H22O2/c1-8(2)13(15)16-12-7-14(9(3)4)6-11(14)10(12)5/h8-9,11-12H,5-7H

InchiKey: CPSOCOUVTGYNEQ-UHFFFAOYSA-N

Formula: C14H22O2

SMILES: C=C1C(OC(=O)C(C)C)CC2(C(C)C)CC12

Mol. weight [g/mol]: 222.32

CAS: 5281-01-6

Physical Properties

Property code	Value	Unit	Source
gf	-10.42	kJ/mol	Joback Method
hf	-362.91	kJ/mol	Joback Method
hfus	17.64	kJ/mol	Joback Method
hvap	53.66	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.176		Crippen Method
mcvol	189.540	ml/mol	McGowan Method
pc	2049.31	kPa	Joback Method
rinpol	1414.00		NIST Webbook
rinpol	1414.00		NIST Webbook
tb	603.34	K	Joback Method
tc	807.74	K	Joback Method
tf	358.92	K	Joback Method
vc	0.727	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.90	J/mol×K	603.34	Joback Method
cpg	535.95	J/mol×K	637.41	Joback Method
cpg	553.01	J/mol×K	671.47	Joback Method
cpg	569.20	J/mol×K	705.54	Joback Method
cpg	584.66	J/mol×K	739.60	Joback Method
cpg	599.50	J/mol×K	773.67	Joback Method
cpg	613.86	J/mol×K	807.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5281016&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

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