Sabinyl propionate

Inchi: InChI=1S/C13H20O2/c1-5-12(14)15-11-7-13(8(2)3)6-10(13)9(11)4/h8,10-11H,4-7H2,1-3
InchiKey: KIVPUZGKBYRCCO-UHFFFAOYSA-N
Formula: C13H20O2
SMILES: C=C1C(OC(=O)CC)CC2(C(C)C)CC12
Mol. weight [g/mol]: 208.30
CAS: 5281-00-5

Physical Properties

Property code	Value	Unit	Source
gf	-16.40	kJ/mol	Joback Method
hf	-336.99	kJ/mol	Joback Method
hfus	18.57	kJ/mol	Joback Method
hvap	51.83	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.930		Crippen Method
mcvol	175.450	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
rinpol	1379.70		NIST Webbook
rinpol	1379.70		NIST Webbook
tb	580.90	K	Joback Method
tc	784.27	K	Joback Method
tf	362.65	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.58	J/mol×K	580.90	Joback Method
cpg	483.76	J/mol×K	614.80	Joback Method
cpg	499.96	J/mol×K	648.69	Joback Method
cpg	515.30	J/mol×K	682.59	Joback Method
cpg	529.90	J/mol×K	716.48	Joback Method
cpg	543.89	J/mol×K	750.38	Joback Method
cpg	557.39	J/mol×K	784.27	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5281005&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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