Sabinol, 3-methylbut-2-enoate

Inchi: InChI=1S/C15H22O2/c1-9(2)6-14(16)17-13-8-15(10(3)4)7-12(15)11(13)5/h6,10,12-13H,5
InchiKey: INAONURJJZWGCJ-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: C=C1C(OC(=O)C=C(C)C)CC2(C(C)C)CC12
Mol. weight [g/mol]: 234.33

Physical Properties

Property code	Value	Unit	Source
gf	72.11	kJ/mol	Joback Method
hf	-270.84	kJ/mol	Joback Method
hfus	22.65	kJ/mol	Joback Method
hvap	56.31	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.487		Crippen Method
mcvol	199.330	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	1614.30		NIST Webbook
rinpol	1614.30		NIST Webbook
tb	630.70	K	Joback Method
tc	839.57	K	Joback Method
tf	366.15	K	Joback Method
vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.97	J/mol×K	630.70	Joback Method
cpg	566.88	J/mol×K	665.51	Joback Method
cpg	583.83	J/mol×K	700.32	Joback Method
cpg	599.97	J/mol×K	735.13	Joback Method
cpg	615.45	J/mol×K	769.95	Joback Method
cpg	630.42	J/mol×K	804.76	Joback Method
cpg	645.03	J/mol×K	839.57	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=U413837&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