Isoverbenyl acetate

Inchi: InChI=1S/C12H18O2/c1-7-5-11(14-8(2)13)10-6-9(7)12(10,3)4/h5,9-11H,6H2,1-4H3/t9-,1
InchiKey: OZBFUQLOVFXDNK-AXFHLTTASA-N
Formula: C12H18O2
SMILES: CC(=O)OC1C=C(C)C2CC1C2(C)C
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	-74.94	kJ/mol	Joback Method
hf	-375.50	kJ/mol	Joback Method
hfus	20.47	kJ/mol	Joback Method
hvap	50.64	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1308.00		NIST Webbook
tb	563.04	K	Joback Method
tc	773.40	K	Joback Method
tf	358.22	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.92	J/mol×K	563.04	Joback Method
cpg	437.32	J/mol×K	598.10	Joback Method
cpg	453.71	J/mol×K	633.16	Joback Method
cpg	469.20	J/mol×K	668.22	Joback Method
cpg	483.90	J/mol×K	703.28	Joback Method
cpg	497.94	J/mol×K	738.34	Joback Method
cpg	511.43	J/mol×K	773.40	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=R568002&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

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