cis-Sabinene hydrate acetate

Inchi: InChI=1S/C12H20O2/c1-8(2)12-6-5-11(4,10(12)7-12)14-9(3)13/h8,10H,5-7H2,1-4H3/t10-

InchiKey: MYCFGFMJUUNKBN-GRYCIOLGSA-N

Formula: C12H20O2

SMILES: CC(=O)OC1(C)CCC2(C(C)C)CC12

Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-83.39	kJ/mol	Joback Method
hf	-385.35	kJ/mol	Joback Method
hfus	10.84	kJ/mol	Joback Method
hvap	48.29	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.764		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	1203.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1206.00		NIST Webbook
tb	559.10	K	Joback Method
tc	772.02	K	Joback Method
tf	361.60	K	Joback Method
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.10	J/mol×K	559.10	Joback Method
cpg	453.75	J/mol×K	594.59	Joback Method
cpg	470.23	J/mol×K	630.07	Joback Method
cpg	485.75	J/mol×K	665.56	Joback Method
cpg	500.56	J/mol×K	701.04	Joback Method
cpg	514.85	J/mol×K	736.53	Joback Method
cpg	528.87	J/mol×K	772.02	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=R603511&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