cis-terpenyl acetate

Inchi: InChI=1S/C12H20O2/c1-9(2)11-5-7-12(4,8-6-11)14-10(3)13/h11H,1,5-8H2,2-4H3/t11-,12

InchiKey: URVNHQCLMBMWIW-TXEJJXNPSA-N

Formula: C12H20O2

SMILES: C=C(C)C1CCC(C)(OC(C)=O)CC1

Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-93.22	kJ/mol	Joback Method
hf	-370.95	kJ/mol	Joback Method
hfus	13.64	kJ/mol	Joback Method
hvap	49.84	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.075		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1350.00		NIST Webbook
tb	561.93	K	Joback Method
tc	777.04	K	Joback Method
tf	308.48	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.60	J/mol×K	561.93	Joback Method
cpg	452.75	J/mol×K	597.78	Joback Method
cpg	470.80	J/mol×K	633.63	Joback Method
cpg	487.86	J/mol×K	669.48	Joback Method
cpg	504.03	J/mol×K	705.33	Joback Method
cpg	519.41	J/mol×K	741.19	Joback Method
cpg	534.10	J/mol×K	777.04	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=R506188&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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