cis-«beta»-terpinyl 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-HAQNSBGRSA-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
hfus	13.64	kJ/mol	Joback Method
hvap	64.43	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
logp	3.075		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
rinpol	1240.00		NIST Webbook
ripol	1622.00		NIST Webbook
ripol	1622.00		NIST Webbook
tf	251.58	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R134040&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point