

cis-Dihydro-«alpha»-terpinyl acetate

Inchi:	InChI=1S/C12H22O2/c1-9-5-7-11(8-6-9)12(3,4)14-10(2)13/h9,11H,5-8H2,1-4H3/t9-,11+
InchiKey:	HBNHCGDYBYBMKJN-JGZJWPJOSA-N
Formula:	C12H22O2
SMILES:	CC(=O)OC(C)(C)C1CCC(C)CC1
Mol. weight [g/mol]:	198.30

Physical Properties

Property code	Value	Unit	Source
hf	-566.64	kJ/mol	Cheméo Relay (1.0)
hfus	15.12	kJ/mol	Joback Method
hvap	62.78	kJ/mol	Cheméo Relay (1.0)
logp	3.154		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2197.95	kPa	Joback Method
rinpol	1298.00		NIST Webbook
tb	496.38	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.11	J/mol×K	561.90	Joback Method
cpg	478.84	J/mol×K	597.12	Joback Method
cpg	498.39	J/mol×K	632.35	Joback Method
cpg	516.77	J/mol×K	667.57	Joback Method
cpg	534.02	J/mol×K	702.79	Joback Method
cpg	550.18	J/mol×K	738.01	Joback Method
cpg	565.28	J/mol×K	773.24	Joback Method
dvisc	0.0039043	Pa×s	302.72	Joback Method
dvisc	0.0017642	Pa×s	345.92	Joback Method
dvisc	0.0009509	Pa×s	389.11	Joback Method
dvisc	0.0005799	Pa×s	432.31	Joback Method
dvisc	0.0003869	Pa×s	475.51	Joback Method
dvisc	0.0002762	Pa×s	518.70	Joback Method
dvisc	0.0002076	Pa×s	561.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R606961&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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