«alpha»-Terpinyl acetate

Other names:	Terpineol, acetate
	p-ment-1-en-8-yl acetate
Inchi:	InChI=1S/C12H20O2/c1-9-5-7-11(8-6-9)12(3,4)14-10(2)13/h5,11H,6-8H2,1-4H3
InchiKey:	IGODOXYLBBXFDW-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	CC(=O)OC(C)(C)C1CC=C(C)CC1
Mol. weight [g/mol]:	196.29
CAS:	8007-35-0

Physical Properties

Property code	Value	Unit	Source
gf	-136.14	kJ/mol	Joback Method
hf	-443.93	kJ/mol	Joback Method
hfus	14.88	kJ/mol	Joback Method
hvap	51.55	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.075		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	1350.00		NIST Webbook
rinpol	1329.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1354.00		NIST Webbook
rinpol	1356.00		NIST Webbook
rinpol	1333.00		NIST Webbook
rinpol	1351.00		NIST Webbook
rinpol	1350.00		NIST Webbook
rinpol	1350.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1709.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1709.00		NIST Webbook
tb	570.71	K	Joback Method
tc	785.17	K	Joback Method
tf	320.24	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.09	J/mol×K	570.71	Joback Method
cpg	456.93	J/mol×K	606.45	Joback Method
cpg	474.66	J/mol×K	642.20	Joback Method
cpg	491.30	J/mol×K	677.94	Joback Method
cpg	506.89	J/mol×K	713.68	Joback Method
cpg	521.47	J/mol×K	749.42	Joback Method
cpg	535.06	J/mol×K	785.17	Joback Method
dvisc	0.0029306	Pa×s	320.24	Joback Method
dvisc	0.0014126	Pa×s	361.99	Joback Method
dvisc	0.0007919	Pa×s	403.73	Joback Method
dvisc	0.0004947	Pa×s	445.48	Joback Method
dvisc	0.0003350	Pa×s	487.22	Joback Method
dvisc	0.0002413	Pa×s	528.97	Joback Method
dvisc	0.0001823	Pa×s	570.71	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C8007350&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume