

m-«alpha»-Terpineol, acetate

Inchi:	InChI=1S/C12H20O2/c1-9-6-5-7-11(8-9)12(3,4)14-10(2)13/h8,11H,5-7H2,1-4H3
InchiKey:	VQUFSEQEIRRWLD-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	CC(=O)OC(C)(C)C1C=C(C)CCC1
Mol. weight [g/mol]:	196.29

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
rinsol	1337.00		NIST Webbook
tb	570.71	K	Joback Method
tc	785.17	K	Joback Method
tf	320.24	K	Joback Method
vc	0.639	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.09	J/molxK	570.71	Joback Method
cpg	456.93	J/molxK	606.45	Joback Method
cpg	474.66	J/molxK	642.20	Joback Method
cpg	491.30	J/molxK	677.94	Joback Method
cpg	506.89	J/molxK	713.68	Joback Method
cpg	521.47	J/molxK	749.42	Joback Method
cpg	535.06	J/molxK	785.17	Joback Method
dvisc	0.0029306	Paxs	320.24	Joback Method
dvisc	0.0014126	Paxs	361.99	Joback Method

dvisc	0.0007919	Paxs	403.73	Joback Method
dvisc	0.0004947	Paxs	445.48	Joback Method
dvisc	0.0003350	Paxs	487.22	Joback Method
dvisc	0.0002413	Paxs	528.97	Joback Method
dvisc	0.0001823	Paxs	570.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R546191&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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