1-Terpineol, acetate

Other names: Terpinen-1-yl, acetate
Inchi: InChI=1S/C12H20O2/c1-9(2)11-5-7-12(4,8-6-11)14-10(3)13/h5,9H,6-8H2,1-4H3
InchiKey: HTFJGCGGTGREIF-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: CC(=O)OC1(C)CC=C(C(C)C)CC1
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-146.91	kJ/mol	Joback Method
hf	-425.22	kJ/mol	Joback Method
hfus	12.47	kJ/mol	Joback Method
hvap	51.31	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	3.075		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
tb	573.74	K	Joback Method
tc	788.23	K	Joback Method
tf	326.72	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.00	J/mol×K	573.74	Joback Method
cpg	451.97	J/mol×K	609.49	Joback Method
cpg	468.96	J/mol×K	645.24	Joback Method
cpg	485.04	J/mol×K	680.99	Joback Method
cpg	500.33	J/mol×K	716.73	Joback Method
cpg	514.91	J/mol×K	752.48	Joback Method
cpg	528.89	J/mol×K	788.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R129796&Units=SI
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

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