4-Terpinenyl acetate

Other names:	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, acetate
	p-Menth-1-en-4-ol, acetate
	Terpinene 4-acetate
	1-Terpinen-4-ol acetate
	4-Terpineol acetate
	Terpin-4-yl acetate
	Terpinen-4-ol, acetate
	Terpinen-4-yl acetate
	Terpinene-4-yl acetate
	1-(Isopropyl)-4-methylcyclohex-3-en-1-yl acetate
	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, 1-acetate
	Menthyl-1-en-4-ol acetate
	Terpin-1-en-4-yl acetate
Inchi:	InChI=1S/C12H20O2/c1-9(2)12(14-11(4)13)7-5-10(3)6-8-12/h5,9H,6-8H2,1-4H3
InchiKey:	BFCBRSFYYLSTAA-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	CC(=O)OC1(C(C)C)CC=C(C)CC1
Mol. weight [g/mol]:	196.29
CAS:	4821-04-9

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	1328.00		NIST Webbook
rinpol	1332.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1331.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1302.00		NIST Webbook

rinpol	1300.00	NIST Webbook
rinpol	1341.00	NIST Webbook
rinpol	1289.00	NIST Webbook
rinpol	1301.00	NIST Webbook
rinpol	1300.00	NIST Webbook
rinpol	1335.00	NIST Webbook
rinpol	1325.00	NIST Webbook
rinpol	1300.00	NIST Webbook
rinpol	1340.00	NIST Webbook
rinpol	1274.00	NIST Webbook
rinpol	1310.00	NIST Webbook
rinpol	1321.00	NIST Webbook
rinpol	1301.00	NIST Webbook
rinpol	1342.00	NIST Webbook
rinpol	1338.00	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1281.00	NIST Webbook
rinpol	1281.00	NIST Webbook
rinpol	1270.00	NIST Webbook
rinpol	1340.00	NIST Webbook
rinpol	1296.00	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1340.00	NIST Webbook
rinpol	1321.00	NIST Webbook
rinpol	1265.00	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1282.00	NIST Webbook
rinpol	1332.00	NIST Webbook
rinpol	1304.00	NIST Webbook
rinpol	1290.00	NIST Webbook
rinpol	1304.00	NIST Webbook
ripol	1640.00	NIST Webbook
ripol	1666.00	NIST Webbook
ripol	1666.00	NIST Webbook
ripol	1609.00	NIST Webbook
ripol	1630.00	NIST Webbook
ripol	1630.00	NIST Webbook
ripol	1628.00	NIST Webbook
ripol	1628.00	NIST Webbook
ripol	1628.00	NIST Webbook
ripol	1640.00	NIST Webbook
ripol	1666.00	NIST Webbook
ripol	1619.00	NIST Webbook
ripol	1640.00	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

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=C4821049&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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