iso-3-Thujyl acetate

Other names:	Isothujyl acetate
	Neo-3-Thujyl alcohol, acetate
	Iso-3-Thujyl alcohol, acetate
	isothujyl-3-acetate
	Thujyl acetate(3-iso)
Inchi:	InChI=1S/C12H20O2/c1-7(2)12-5-10(12)8(3)11(6-12)14-9(4)13/h7-8,10-11H,5-6H2,1-4H
InchiKey:	RYMWIDNPMDLHRP-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	CC(=O)OC1CC2(C(C)C)CC2C1C
Mol. weight [g/mol]:	196.29
CAS:	62181-90-2

Physical Properties

Property code	Value	Unit	Source
gf	-85.61	kJ/mol	Joback Method
hf	-420.93	kJ/mol	Joback Method
hfus	18.21	kJ/mol	Joback Method
hvap	49.13	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.620		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2318.07	kPa	Joback Method
rinpol	1301.00		NIST Webbook
rinpol	1273.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1266.50		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1266.50		NIST Webbook

rinpol	1301.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1291.00		NIST Webbook
ripol	1630.00		NIST Webbook
tb	554.19	K	Joback Method
tc	758.84	K	Joback Method
tf	333.46	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.10	J/mol×K	554.19	Joback Method
cpg	456.42	J/mol×K	588.30	Joback Method
cpg	473.65	J/mol×K	622.41	Joback Method
cpg	489.90	J/mol×K	656.52	Joback Method
cpg	505.31	J/mol×K	690.62	Joback Method
cpg	519.99	J/mol×K	724.73	Joback Method
cpg	534.06	J/mol×K	758.84	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62181902&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume