

neo-iso-3-Thujyl acetate

Other names:	Neo-iso-3-Thujyl alcohol, acetate
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:	62181-91-3

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	1268.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1268.00		NIST Webbook
rinpol	1268.00		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/molxK	554.19	Joback Method
cpg	456.42	J/molxK	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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C62181913&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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