

neo-iso-3-Thujyl 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-VJPOPMDVSA-N
Formula:	C12H20O2
SMILES:	CC(=O)OC1CC2(C(C)C)CC2C1C
Mol. weight [g/mol]:	196.29

Physical Properties

Property code	Value	Unit	Source
hfus	18.21	kJ/mol	Joback Method
logp	2.620		Crippen Method
mcvol	165.660	ml/mol	McGowan 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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R603640&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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