Nojigiku acetate

Other names: Nojigiku acetate
Inchi: InChI=1S/C12H18O2/c1-7-10-5-9(12(7,3)4)6-11(10)14-8(2)13/h9-11H,1,5-6H2,2-4H3
InchiKey: GVZSSHYAFJPRJY-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: C=C1C2CC(CC2OC(C)=O)C1(C)C
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
hfus	18.48	kJ/mol	Joback Method
logp	2.540		Crippen Method
mcvol	161.360	ml/mol	McGowan Method
rinpol	1272.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.91	J/mol×K	558.06	Joback Method
cpg	436.52	J/mol×K	592.92	Joback Method
cpg	453.10	J/mol×K	627.77	Joback Method
cpg	468.76	J/mol×K	662.63	Joback Method
cpg	483.62	J/mol×K	697.48	Joback Method
cpg	497.79	J/mol×K	732.34	Joback Method
cpg	511.38	J/mol×K	767.19	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55627026&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.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

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