cis-Pinocarvyl acetate

Other names: cis-Pinocarveol, acetate
Inchi: InChI=1S/C12H18O2/c1-7-10-5-9(12(10,3)4)6-11(7)14-8(2)13/h9-11H,1,5-6H2,2-4H3/t9-
InchiKey: UDBAGFUFASPUFS-AXFHLTTASA-N
Formula: C12H18O2
SMILES: C=C1C(OC(C)=O)CC2CC1C2(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	1309.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1299.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1312.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1301.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1301.00		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

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R121014&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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