Filifolide A

Inchi: InChI=1S/C10H14O2/c1-6-5-10(2,3)7-4-8(6)12-9(7)11/h5,7-8H,4H2,1-3H3
InchiKey: JHKNAYGQYUKKDQ-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC1=CC(C)(C)C2CC1OC2=O
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	-70.96	kJ/mol	Joback Method
hf	-344.94	kJ/mol	Joback Method
hfus	16.82	kJ/mol	Joback Method
hvap	46.28	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.904		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	3055.79	kPa	Joback Method
ripol	1996.00		NIST Webbook
tb	544.70	K	Joback Method
tc	777.48	K	Joback Method
tf	359.03	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.26	J/mol×K	544.70	Joback Method
cpg	355.17	J/mol×K	583.50	Joback Method
cpg	371.01	J/mol×K	622.29	Joback Method
cpg	385.92	J/mol×K	661.09	Joback Method
cpg	400.04	J/mol×K	699.89	Joback Method
cpg	413.48	J/mol×K	738.69	Joback Method
cpg	426.39	J/mol×K	777.48	Joback Method

Sources

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=R336499&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/75-956-8/Filifolide-A.pdf

Generated by Cheméo on 2024-10-12 09:41:03.644929921 +0000 UTC m=+3306926.281899170.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.