Ethyl 2-(5-methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl carbonate

Inchi: InChI=1S/C13H22O4/c1-6-13(5)9-8-10(16-13)12(3,4)17-11(14)15-7-2/h6,10H,1,7-9H2,2-

InchiKey: HRYCRSVSFJLRBW-UHFFFAOYSA-N

Formula: C13H22O4

SMILES: C=CC1(C)CCC(C(C)(C)OC(=O)OCC)O1

Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	-252.43	kJ/mol	Joback Method
hf	-648.61	kJ/mol	Joback Method
hfus	21.39	kJ/mol	Joback Method
hvap	57.44	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.062		Crippen Method
mcvol	198.050	ml/mol	McGowan Method
pc	2079.33	kPa	Joback Method
rinpol	1090.00		NIST Webbook
tb	626.80	K	Joback Method
tc	835.75	K	Joback Method
tf	388.45	K	Joback Method
vc	0.735	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.48	J/mol×K	626.80	Joback Method
cpg	565.54	J/mol×K	661.63	Joback Method
cpg	582.62	J/mol×K	696.45	Joback Method
cpg	598.82	J/mol×K	731.28	Joback Method
cpg	614.25	J/mol×K	766.10	Joback Method
cpg	629.01	J/mol×K	800.93	Joback Method
cpg	643.21	J/mol×K	835.75	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=U373803&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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