2-(5-Methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C17H17F5O3/c1-5-17(4)7-6-8(24-17)16(2,3)25-15(23)9-10(18)12(20)14(22)13

InchiKey: LXPIGNHRJUAYHQ-UHFFFAOYSA-N

Formula: C17H17F5O3

SMILES: C=CC1(C)CCC(C(C)(C)OC(=O)c2c(F)c(F)c(F)c(F)c2F)O1

Mol. weight [g/mol]: 364.31

Physical Properties

Property code	Value	Unit	Source
gf	-1023.54	kJ/mol	Joback Method
hf	-1400.32	kJ/mol	Joback Method
hfus	38.06	kJ/mol	Joback Method
hvap	65.43	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	4.441		Crippen Method
mcvol	233.630	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	1667.00		NIST Webbook
rinpol	1667.00		NIST Webbook
tb	743.83	K	Joback Method
tc	942.85	K	Joback Method
tf	503.27	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.88	J/mol×K	743.83	Joback Method
cpg	705.95	J/mol×K	777.00	Joback Method
cpg	720.37	J/mol×K	810.17	Joback Method
cpg	734.25	J/mol×K	843.34	Joback Method
cpg	747.66	J/mol×K	876.51	Joback Method
cpg	760.73	J/mol×K	909.68	Joback Method
cpg	773.54	J/mol×K	942.85	Joback Method

Sources

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=U373604&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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