2-(5-Methyl-5-vinyltetrahydrofuran-2-yl)propan-2-yl 3-chlorobenzoate

Inchi: InChI=1S/C17H21ClO3/c1-5-17(4)10-9-14(20-17)16(2,3)21-15(19)12-7-6-8-13(18)11-12/
InchiKey: NWVWKPPRSHNJPP-UHFFFAOYSA-N
Formula: C17H21ClO3
SMILES: C=CC1(C)CCC(C(C)(C)OC(=O)c2cccc(Cl)c2)O1
Mol. weight [g/mol]: 308.80

Physical Properties

Property code	Value	Unit	Source
gf	-22.90	kJ/mol	Joback Method
hf	-389.63	kJ/mol	Joback Method
hfus	28.41	kJ/mol	Joback Method
hvap	71.26	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.399		Crippen Method
mcvol	237.020	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinpol	2024.00		NIST Webbook
rinpol	2024.00		NIST Webbook
tb	764.99	K	Joback Method
tc	1005.35	K	Joback Method
tf	480.16	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.15	J/mol×K	764.99	Joback Method
cpg	701.18	J/mol×K	805.05	Joback Method
cpg	718.36	J/mol×K	845.11	Joback Method
cpg	734.87	J/mol×K	885.17	Joback Method
cpg	750.92	J/mol×K	925.23	Joback Method
cpg	766.72	J/mol×K	965.29	Joback Method
cpg	782.47	J/mol×K	1005.35	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=U373576&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

Latest version available from:
https://www.chemeo.com/cid/52-527-9/2-5-Methyl-5-vinyltetrahydrofuran-2-yl-propan-2-yl-3-chlorobenzoate.pdf
Generated by Cheméo on 2024-04-29 14:53:31.732672312 +0000 UTC m=+16691660.653249627.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.