1-(tert-Butoxy)propan-2-yl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C14H15F5O3/c1-6(5-21-14(2,3)4)22-13(20)7-8(15)10(17)12(19)11(18)9(7)16/h

InchiKey: MBGGJCWXZKBQBZ-UHFFFAOYSA-N

Formula: C14H15F5O3

SMILES: CC(COC(C)(C)C)OC(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 326.26

Physical Properties

Property code	Value	Unit	Source
gf	-1181.31	kJ/mol	Joback Method
hf	-1524.71	kJ/mol	Joback Method
hfus	32.55	kJ/mol	Joback Method
hvap	58.14	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.742		Crippen Method
mcvol	206.520	ml/mol	McGowan Method
pc	1632.49	kPa	Joback Method
rinpol	1439.00		NIST Webbook
rinpol	1439.00		NIST Webbook
tb	662.69	K	Joback Method
tc	841.51	K	Joback Method
tf	421.32	K	Joback Method
vc	0.827	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.13	J/mol×K	662.69	Joback Method
cpg	575.09	J/mol×K	692.49	Joback Method
cpg	587.40	J/mol×K	722.30	Joback Method
cpg	599.04	J/mol×K	752.10	Joback Method
cpg	610.04	J/mol×K	781.91	Joback Method
cpg	620.39	J/mol×K	811.71	Joback Method
cpg	630.10	J/mol×K	841.51	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=U378319&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