1-(tert-Butoxy)propan-2-yl 2,2,3,3,3-pentafluoropropanoate

Inchi: InChI=1S/C10H15F5O3/c1-6(5-17-8(2,3)4)18-7(16)9(11,12)10(13,14)15/h6H,5H2,1-4H3

InchiKey: VZXDHJSIRZCDHL-UHFFFAOYSA-N

Formula: C10H15F5O3

SMILES: CC(COC(C)(C)C)OC(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 278.22

Physical Properties

Property code	Value	Unit	Source
gf	-1273.57	kJ/mol	Joback Method
hf	-1638.83	kJ/mol	Joback Method
hfus	15.27	kJ/mol	Joback Method
hvap	41.06	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.931		Crippen Method
mcvol	173.920	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	945.00		NIST Webbook
rinpol	945.00		NIST Webbook
tb	513.13	K	Joback Method
tc	677.43	K	Joback Method
tf	292.06	K	Joback Method
vc	0.689	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.37	J/mol×K	513.13	Joback Method
cpg	458.28	J/mol×K	540.51	Joback Method
cpg	471.43	J/mol×K	567.90	Joback Method
cpg	483.86	J/mol×K	595.28	Joback Method
cpg	495.59	J/mol×K	622.66	Joback Method
cpg	506.66	J/mol×K	650.05	Joback Method
cpg	517.08	J/mol×K	677.43	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=U378328&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