1-tert-Butoxy-2-propanol, trifluoroacetate

Inchi: InChI=1S/C9H15F3O3/c1-6(5-14-8(2,3)4)15-7(13)9(10,11)12/h6H,5H2,1-4H3
InchiKey: KQUKTGUJHIFMOJ-UHFFFAOYSA-N
Formula: C9H15F3O3
SMILES: CC(COC(C)(C)C)OC(=O)C(F)(F)F
Mol. weight [g/mol]: 228.21

Physical Properties

Property code	Value	Unit	Source
gf	-895.21	kJ/mol	Joback Method
hf	-1217.22	kJ/mol	Joback Method
hfus	13.93	kJ/mol	Joback Method
hvap	41.76	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.296		Crippen Method
mcvol	156.290	ml/mol	McGowan Method
pc	2179.52	kPa	Joback Method
rinpol	878.00		NIST Webbook
rinpol	878.00		NIST Webbook
tb	494.94	K	Joback Method
tc	666.54	K	Joback Method
tf	277.19	K	Joback Method
vc	0.608	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.86	J/mol×K	494.94	Joback Method
cpg	392.35	J/mol×K	523.54	Joback Method
cpg	405.18	J/mol×K	552.14	Joback Method
cpg	417.36	J/mol×K	580.74	Joback Method
cpg	428.92	J/mol×K	609.34	Joback Method
cpg	439.87	J/mol×K	637.94	Joback Method
cpg	450.24	J/mol×K	666.54	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376272&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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