4-(Trifluoroacetyloxy)benzoic trifluoroacetic anhydride

Inchi: InChI=1S/C11H4F6O5/c12-10(13,14)8(19)21-6-3-1-5(2-4-6)7(18)22-9(20)11(15,16)17/h1
InchiKey: UPIJEAGCYJIKHJ-UHFFFAOYSA-N
Formula: C11H4F6O5
SMILES: O=C(OC(=O)C(F)(F)F)c1ccc(OC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 330.14

Physical Properties

Property code	Value	Unit	Source
gf	-1615.42	kJ/mol	Joback Method
hf	-1841.65	kJ/mol	Joback Method
hfus	28.72	kJ/mol	Joback Method
hvap	60.58	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.400		Crippen Method
mcvol	169.160	ml/mol	McGowan Method
pc	2414.74	kPa	Joback Method
rinpol	1174.00		NIST Webbook
rinpol	1174.00		NIST Webbook
tb	678.35	K	Joback Method
tc	870.39	K	Joback Method
tf	455.30	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.42	J/mol×K	678.35	Joback Method
cpg	463.37	J/mol×K	710.36	Joback Method
cpg	471.57	J/mol×K	742.36	Joback Method
cpg	479.08	J/mol×K	774.37	Joback Method
cpg	485.91	J/mol×K	806.38	Joback Method
cpg	492.10	J/mol×K	838.38	Joback Method
cpg	497.67	J/mol×K	870.39	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=U375071&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