Benzoic acid, 3-(trifluoroacetyloxy)-

Inchi: InChI=1S/C9H5F3O4/c10-9(11,12)8(15)16-6-3-1-2-5(4-6)7(13)14/h1-4H,(H,13,14)
InchiKey: NFPLYVXJTDHGFA-UHFFFAOYSA-N
Formula: C9H5F3O4
SMILES: O=C(O)c1cccc(OC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 234.13

Physical Properties

Property code	Value	Unit	Source
gf	-953.57	kJ/mol	Joback Method
hf	-1110.72	kJ/mol	Joback Method
hfus	23.02	kJ/mol	Joback Method
hvap	67.40	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	1.853		Crippen Method
mcvol	134.100	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	1324.00		NIST Webbook
rinpol	1324.00		NIST Webbook
tb	653.90	K	Joback Method
tc	848.20	K	Joback Method
tf	417.23	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.43	J/mol×K	653.90	Joback Method
cpg	349.42	J/mol×K	686.28	Joback Method
cpg	356.82	J/mol×K	718.67	Joback Method
cpg	363.65	J/mol×K	751.05	Joback Method
cpg	369.94	J/mol×K	783.43	Joback Method
cpg	375.72	J/mol×K	815.82	Joback Method
cpg	381.00	J/mol×K	848.20	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375036&Units=SI

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

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