Benzoic acid, 2-(trifluoroacetylthio)-, methyl ester

Inchi: InChI=1S/C10H7F3O3S/c1-16-8(14)6-4-2-3-5-7(6)17-9(15)10(11,12)13/h2-5H,1H3
InchiKey: KZDAPZDUVLDWOO-UHFFFAOYSA-N
Formula: C10H7F3O3S
SMILES: COC(=O)c1ccccc1SC(=O)C(F)(F)F
Mol. weight [g/mol]: 264.22

Physical Properties

Property code	Value	Unit	Source
gf	-775.21	kJ/mol	Joback Method
hf	-937.26	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	59.76	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.654		Crippen Method
mcvol	158.670	ml/mol	McGowan Method
pc	2915.53	kPa	Joback Method
rinpol	1390.00		NIST Webbook
rinpol	1390.00		NIST Webbook
tb	653.38	K	Joback Method
tc	873.50	K	Joback Method
tf	402.08	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.71	J/mol×K	653.38	Joback Method
cpg	401.29	J/mol×K	690.07	Joback Method
cpg	411.02	J/mol×K	726.75	Joback Method
cpg	419.92	J/mol×K	763.44	Joback Method
cpg	428.03	J/mol×K	800.12	Joback Method
cpg	435.37	J/mol×K	836.81	Joback Method
cpg	441.97	J/mol×K	873.50	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=U375163&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