Benzoic acid, 3-(trifluoroacetylthio)-

Inchi: InChI=1S/C9H5F3O3S/c10-9(11,12)8(15)16-6-3-1-2-5(4-6)7(13)14/h1-4H,(H,13,14)
InchiKey: PFYMLSCEXRUNLX-UHFFFAOYSA-N
Formula: C9H5F3O3S
SMILES: O=C(O)c1cccc(SC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 250.19

Physical Properties

Property code	Value	Unit	Source
gf	-815.45	kJ/mol	Joback Method
hf	-936.63	kJ/mol	Joback Method
hfus	25.96	kJ/mol	Joback Method
hvap	71.81	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.566		Crippen Method
mcvol	144.580	ml/mol	McGowan Method
pc	3686.49	kPa	Joback Method
rinpol	1504.00		NIST Webbook
rinpol	1504.00		NIST Webbook
tb	700.26	K	Joback Method
tc	910.85	K	Joback Method
tf	429.40	K	Joback Method
vc	0.559	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.74	J/mol×K	700.26	Joback Method
cpg	369.39	J/mol×K	735.36	Joback Method
cpg	376.37	J/mol×K	770.46	Joback Method
cpg	382.71	J/mol×K	805.55	Joback Method
cpg	388.45	J/mol×K	840.65	Joback Method
cpg	393.64	J/mol×K	875.75	Joback Method
cpg	398.30	J/mol×K	910.85	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=U375175&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