3-(Trifluoroacetylthio)benzoyl chloride

Inchi: InChI=1S/C9H4ClF3O2S/c10-7(14)5-2-1-3-6(4-5)16-8(15)9(11,12)13/h1-4H
InchiKey: SWCJJWCTMSHJJS-UHFFFAOYSA-N
Formula: C9H4ClF3O2S
SMILES: O=C(Cl)c1cccc(SC(=O)C(F)(F)F)c1
Mol. weight [g/mol]: 268.64

Physical Properties

Property code	Value	Unit	Source
gf	-690.56	kJ/mol	Joback Method
hf	-800.14	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	59.51	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.247		Crippen Method
mcvol	150.950	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	1391.00		NIST Webbook
rinpol	1391.00		NIST Webbook
tb	645.51	K	Joback Method
tc	876.00	K	Joback Method
tf	398.50	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.35	J/mol×K	645.51	Joback Method
cpg	351.35	J/mol×K	683.92	Joback Method
cpg	359.50	J/mol×K	722.34	Joback Method
cpg	366.85	J/mol×K	760.75	Joback Method
cpg	373.44	J/mol×K	799.17	Joback Method
cpg	379.34	J/mol×K	837.58	Joback Method
cpg	384.58	J/mol×K	876.00	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=U375150&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