2-(Trifluoromethyl)thiophenol, S-acetyl-

Inchi: InChI=1S/C9H7F3OS/c1-6(13)14-8-5-3-2-4-7(8)9(10,11)12/h2-5H,1H3
InchiKey: ASPOUDUPCPIORC-UHFFFAOYSA-N
Formula: C9H7F3OS
SMILES: CC(=O)Sc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 220.21

Physical Properties

Property code	Value	Unit	Source
gf	-549.71	kJ/mol	Joback Method
hf	-671.82	kJ/mol	Joback Method
hfus	20.27	kJ/mol	Joback Method
hvap	48.38	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.344		Crippen Method
mcvol	137.140	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1243.20		NIST Webbook
tb	554.21	K	Joback Method
tc	773.76	K	Joback Method
tf	318.65	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.27	J/mol×K	554.21	Joback Method
cpg	320.84	J/mol×K	590.80	Joback Method
cpg	331.54	J/mol×K	627.39	Joback Method
cpg	341.39	J/mol×K	663.99	Joback Method
cpg	350.45	J/mol×K	700.58	Joback Method
cpg	358.76	J/mol×K	737.17	Joback Method
cpg	366.37	J/mol×K	773.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353094&Units=SI
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

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