4-(Methylmercapto)phenol, trifluoroacetate

Other names: 4-(methylthio)phenol
Inchi: InChI=1S/C9H7F3O2S/c1-15-7-4-2-6(3-5-7)14-8(13)9(10,11)12/h2-5H,1H3
InchiKey: JESYZQRXGKWXAQ-UHFFFAOYSA-N
Formula: C9H7F3O2S
SMILES: CSc1ccc(OC(=O)C(F)(F)F)cc1
Mol. weight [g/mol]: 236.21

Physical Properties

Property code	Value	Unit	Source
gf	-654.71	kJ/mol	Joback Method
hf	-804.04	kJ/mol	Joback Method
hfus	21.46	kJ/mol	Joback Method
hvap	50.79	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	2.876		Crippen Method
mcvol	143.010	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1230.00		NIST Webbook
rinpol	1230.00		NIST Webbook
tb	576.63	K	Joback Method
tc	793.57	K	Joback Method
tf	340.88	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.93	J/mol×K	576.63	Joback Method
cpg	343.21	J/mol×K	612.79	Joback Method
cpg	353.69	J/mol×K	648.94	Joback Method
cpg	363.39	J/mol×K	685.10	Joback Method
cpg	372.34	J/mol×K	721.26	Joback Method
cpg	380.55	J/mol×K	757.41	Joback Method
cpg	388.07	J/mol×K	793.57	Joback Method

Sources

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=U353189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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