m-Trifluoromethylthiophenol

Other names:	3-Trifluoromethylthiophenol
	3-Trifluoromethylbenzenethiol
Inchi:	InChI=1S/C7H5F3S/c8-7(9,10)5-2-1-3-6(11)4-5/h1-4,11H
InchiKey:	SCURCOWZQJIUGR-UHFFFAOYSA-N
Formula:	C7H5F3S
SMILES:	FC(F)(F)c1cccc(S)c1
Mol. weight [g/mol]:	178.18
CAS:	937-00-8

Physical Properties

Property code	Value	Unit	Source
gf	-441.36	kJ/mol	Joback Method
hf	-521.35	kJ/mol	Joback Method
hfus	13.41	kJ/mol	Joback Method
hvap	37.10	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.994		Crippen Method
mcvol	107.390	ml/mol	McGowan Method
pc	3782.33	kPa	Joback Method
tb	448.66	K	Joback Method
tc	665.74	K	Joback Method
tf	248.24	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.59	J/mol×K	448.66	Joback Method
cpg	220.48	J/mol×K	484.84	Joback Method
cpg	230.54	J/mol×K	521.02	Joback Method
cpg	239.79	J/mol×K	557.20	Joback Method
cpg	248.30	J/mol×K	593.38	Joback Method
cpg	256.11	J/mol×K	629.56	Joback Method
cpg	263.27	J/mol×K	665.74	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=C937008&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume