3-(Trifluoromethyl)thiophenol

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

Physical Properties

Property code	Value	Unit	Source
hf	-580.93	kJ/mol	Cheméo Relay (1.0)
hfus	13.41	kJ/mol	Joback Method
hvap	49.60	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-2.70		Cheméo Relay (1.0)
logp	2.994		Crippen Method
mcvol	107.390	ml/mol	McGowan Method
tb	445.59	K	Cheméo Relay (1.0)
tc	653.08	K	Cheméo Relay (1.0)
tf	284.11	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C937008&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point