2-(Trifluoromethyl)thiophenol, S-methyl-

Inchi: InChI=1S/C8H7F3S/c1-12-7-5-3-2-4-6(7)8(9,10)11/h2-5H,1H3
InchiKey: DZBNBTCLFBOHJR-UHFFFAOYSA-N
Formula: C8H7F3S
SMILES: CSc1ccccc1C(F)(F)F
Mol. weight [g/mol]: 192.20

Physical Properties

Property code	Value	Unit	Source
gf	-429.21	kJ/mol	Joback Method
hf	-538.60	kJ/mol	Joback Method
hfus	16.08	kJ/mol	Joback Method
hvap	39.41	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.427		Crippen Method
mcvol	121.480	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	1152.10		NIST Webbook
tb	477.46	K	Joback Method
tc	691.26	K	Joback Method
tf	257.45	K	Joback Method
vc	0.472	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.34	J/mol×K	477.46	Joback Method
cpg	263.35	J/mol×K	513.09	Joback Method
cpg	274.52	J/mol×K	548.73	Joback Method
cpg	284.89	J/mol×K	584.36	Joback Method
cpg	294.49	J/mol×K	619.99	Joback Method
cpg	303.37	J/mol×K	655.63	Joback Method
cpg	311.57	J/mol×K	691.26	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=U353095&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