Phenyl trifluoromethyl sulfide

Other names:	Benzene, [(trifluoromethyl)thio]-
	Trifluoromethylthiobenzene
Inchi:	InChI=1S/C7H5F3S/c8-7(9,10)11-6-4-2-1-3-5-6/h1-5H
InchiKey:	YQQKTCBMKQQOSM-UHFFFAOYSA-N
Formula:	C7H5F3S
SMILES:	FC(F)(F)Sc1ccccc1
Mol. weight [g/mol]:	178.18
CAS:	456-56-4

Physical Properties

Property code	Value	Unit	Source
gf	-428.00	kJ/mol	Joback Method
hf	-506.49	kJ/mol	Joback Method
hfus	13.88	kJ/mol	Joback Method
hvap	36.52	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.298		Crippen Method
mcvol	107.390	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
tb	449.60	K	Joback Method
tc	665.13	K	Joback Method
tf	233.66	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.60	J/mol×K	449.60	Joback Method
cpg	222.00	J/mol×K	485.52	Joback Method
cpg	232.54	J/mol×K	521.44	Joback Method
cpg	242.25	J/mol×K	557.37	Joback Method
cpg	251.17	J/mol×K	593.29	Joback Method
cpg	259.35	J/mol×K	629.21	Joback Method
cpg	266.84	J/mol×K	665.13	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C456564&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume