Benzenethiol, pentafluoro-

Other names:	Pentafluorobenzenethiol
	Pentafluorothiophenol
	2,3,4,5,6-Pentafluorothiphenol
Inchi:	InChI=1S/C6HF5S/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H
InchiKey:	UVAMFBJPMUMURT-UHFFFAOYSA-N
Formula:	C6HF5S
SMILES:	Fc1c(F)c(F)c(S)c(F)c1F
Mol. weight [g/mol]:	200.13
CAS:	771-62-0

Physical Properties

Property code	Value	Unit	Source
gf	-880.76	kJ/mol	Joback Method
hf	-930.06	kJ/mol	Joback Method
hfus	22.83	kJ/mol	Joback Method
hvap	37.19	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	2.671		Crippen Method
mcvol	96.840	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
tb	416.00	K	NIST Webbook
tb	416.20	K	NIST Webbook
tc	636.97	K	Joback Method
tf	285.81	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.23	J/mol×K	447.47	Joback Method
cpg	192.07	J/mol×K	479.05	Joback Method
cpg	197.69	J/mol×K	510.64	Joback Method
cpg	203.09	J/mol×K	542.22	Joback Method
cpg	208.26	J/mol×K	573.81	Joback Method

cpg	213.22	J/mol×K	605.39	Joback Method
cpg	217.94	J/mol×K	636.97	Joback Method

Sources

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=C771620&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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