2,3,5,6-TETRAFLUOROTHIOPHENOL

Other names: Benzenethiol, 2,3,5,6-tetrafluoro-
2,3,5,6-tetrafluorobenzenethiol
Inchi: InChI=1S/C6H2F4S/c7-2-1-3(8)5(10)6(11)4(2)9/h1,11H
InchiKey: IGOGJHYWSOZGAE-UHFFFAOYSA-N
Formula: C6H2F4S
SMILES: Fc1cc(F)c(F)c(S)c1F
Mol. weight [g/mol]: 182.14

Physical Properties

Property code	Value	Unit	Source
af	0.3792		Cheméo Relay (1.0)
hf	-596.99	kJ/mol	Cheméo Relay (1.0)
hfus	20.14	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Cheméo Relay (1.0)
ie	9.01	eV	Cheméo Relay (1.0)
log10ws	-3.38		Cheméo Relay (1.0)
logp	2.532		Crippen Method
mcvol	95.070	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	425.70	K	NIST Webbook
tc	632.85	K	Cheméo Relay (1.0)
tf	260.06	K	Cheméo Relay (1.0)
vc	0.344	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	177.91	J/mol×K	443.22	Joback Method
cpg	184.50	J/mol×K	476.32	Joback Method
cpg	190.79	J/mol×K	509.42	Joback Method
cpg	196.80	J/mol×K	542.52	Joback Method
cpg	202.52	J/mol×K	575.62	Joback Method
cpg	207.96	J/mol×K	608.72	Joback Method
cpg	213.12	J/mol×K	641.82	Joback Method

Sources

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=C769404&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume