Sulfur trifluoride

Inchi: InChI=1S/F3S/c1-4(2)3
InchiKey: PSCXEUSWZWRCMQ-UHFFFAOYSA-N
Formula: F3S
SMILES: F[SH](F)F
Mol. weight [g/mol]: 89.06
CAS: 30937-38-3

Physical Properties

Property code	Value	Unit	Source
ea	3.07 ± 0.20	eV	NIST Webbook
ea	2.90 ± 0.10	eV	NIST Webbook
ea	2.50 ± 0.50	eV	NIST Webbook
ea	2.73 ± 0.65	eV	NIST Webbook
ea	2.71	eV	NIST Webbook
gf	-710.68	kJ/mol	Joback Method
hf	-704.80	kJ/mol	Joback Method
hfus	5.67	kJ/mol	Joback Method
hvap	20.17	kJ/mol	Joback Method
ie	7.30	eV	NIST Webbook
ie	8.18 ± 0.07	eV	NIST Webbook
log10ws	-1.54		Crippen Method
logp	1.641		Crippen Method
mcvol	36.820	ml/mol	McGowan Method
pc	5273.90	kPa	Joback Method
tb	261.47	K	Joback Method
tc	423.23	K	Joback Method
vc	0.162	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	61.75	J/mol×K	261.47	Joback Method
cpg	62.16	J/mol×K	288.43	Joback Method
cpg	62.85	J/mol×K	315.39	Joback Method

cpg	63.79	J/mol×K	342.35	Joback Method
cpg	64.96	J/mol×K	369.31	Joback Method
cpg	66.32	J/mol×K	396.27	Joback Method
cpg	67.87	J/mol×K	423.23	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=C30937383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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
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
vc:	Critical Volume