Methane, thiobis[trifluoro-

Other names:	Sulfide, bis(trifluoromethyl)
	Bis(trifluoromethyl) sulfide
	Trifluoromethyl sulfide
	Methane, thiobis*trifluoro-
	Hexafluorodimethyl sulfide
Inchi:	InChI=1S/C2F6S/c3-1(4,5)9-2(6,7)8
InchiKey:	OFHCXWMZXQBQMH-UHFFFAOYSA-N
Formula:	C2F6S
SMILES:	FC(F)(F)SC(F)(F)F
Mol. weight [g/mol]:	170.08
CAS:	371-78-8

Physical Properties

Property code	Value	Unit	Source
gf	-1164.10	kJ/mol	Joback Method
hf	-1236.90	kJ/mol	Joback Method
hfus	8.72	kJ/mol	Joback Method
hvap	19.37	kJ/mol	Joback Method
ie	11.11 ± 0.03	eV	NIST Webbook
ie	11.28 ± 0.04	eV	NIST Webbook
log10ws	-2.86		Crippen Method
logp	2.759		Crippen Method
mcvol	66.010	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	303.10	K	Joback Method
tc	456.31	K	Joback Method
tf	155.08	K	Joback Method
vc	0.287	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	122.83	J/mol×K	303.10	Joback Method
cpg	129.26	J/mol×K	328.64	Joback Method

cpg	135.26	J/mol×K	354.17	Joback Method
cpg	140.85	J/mol×K	379.71	Joback Method
cpg	146.05	J/mol×K	405.24	Joback Method
cpg	150.87	J/mol×K	430.78	Joback Method
cpg	155.33	J/mol×K	456.31	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C371788&Units=SI

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
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