Disulfide, bis(trifluoromethyl)

Other names:	Bis(trifluoromethyl) disulfide
	Di(methyl) disulfide, perfluoro-
	Perfluorodimethyl disulfide
	Trifluoromethyl disulfide
	di(Trifluoromethyl)disulfide
Inchi:	InChI=1S/C2F6S2/c3-1(4,5)9-10-2(6,7)8
InchiKey:	CGMFFOXAQVRUAZ-UHFFFAOYSA-N
Formula:	C2F6S2
SMILES:	FC(F)(F)SSC(F)(F)F
Mol. weight [g/mol]:	202.14
CAS:	372-64-5

Physical Properties

Property code	Value	Unit	Source
gf	-1130.98	kJ/mol	Joback Method
hf	-1195.03	kJ/mol	Joback Method
hfus	12.85	kJ/mol	Joback Method
hvap	26.19	kJ/mol	Joback Method
ie	10.68 ± 0.19	eV	NIST Webbook
ie	10.60 ± 0.03	eV	NIST Webbook
log10ws	-3.73		Crippen Method
logp	3.407		Crippen Method
mcvol	82.360	ml/mol	McGowan Method
pc	3867.48	kPa	Joback Method
tb	307.50 ± 0.50	K	NIST Webbook
tb	307.70	K	NIST Webbook
tc	552.25	K	Joback Method
tf	189.48	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.83	J/mol×K	371.88	Joback Method

cpg	167.44	J/mol×K	401.94	Joback Method
cpg	173.54	J/mol×K	432.00	Joback Method
cpg	179.15	J/mol×K	462.06	Joback Method
cpg	184.29	J/mol×K	492.13	Joback Method
cpg	188.98	J/mol×K	522.19	Joback Method
cpg	193.24	J/mol×K	552.25	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58626e+01
Coeff. B	-3.46042e+03
Temperature range (K), min.	222.18
Temperature range (K), max.	327.97

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C372645&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume