Trisulfide, bis(trifluoromethyl)

Other names:	Bis(trifluoromethyl)trisulfane
	Di(methyl) trisulfide, perfluoro-
Inchi:	InChI=1S/C2F6S3/c3-1(4,5)9-11-10-2(6,7)8
InchiKey:	BHXPRVBRPHEPLQ-UHFFFAOYSA-N
Formula:	C2F6S3
SMILES:	FC(F)(F)SSSC(F)(F)F
Mol. weight [g/mol]:	234.21
CAS:	372-06-5

Physical Properties

Property code	Value	Unit	Source
gf	-1097.86	kJ/mol	Joback Method
hf	-1153.16	kJ/mol	Joback Method
hfus	16.98	kJ/mol	Joback Method
hvap	33.00	kJ/mol	Joback Method
ie	10.16 ± 0.03	eV	NIST Webbook
log10ws	-4.61		Crippen Method
logp	4.056		Crippen Method
mcvol	98.710	ml/mol	McGowan Method
pc	3950.57	kPa	Joback Method
tb	440.66	K	Joback Method
tc	645.88	K	Joback Method
tf	223.88	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.78	J/mol×K	440.66	Joback Method
cpg	204.44	J/mol×K	474.86	Joback Method
cpg	210.51	J/mol×K	509.07	Joback Method
cpg	216.01	J/mol×K	543.27	Joback Method
cpg	220.96	J/mol×K	577.47	Joback Method
cpg	225.40	J/mol×K	611.68	Joback Method

cpg	229.35	J/mol×K	645.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C372065&Units=SI
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume