Carbonotrithioic acid, bis(trifluoromethyl) ester

Other names: Carbonic acid, trithio-, bis(trifluoromethyl) ester
Trithiocarbonic acid, bis(trifluoromethyl) ester
Inchi: InChI=1S/C3F6S3/c4-2(5,6)11-1(10)12-3(7,8)9
InchiKey: BHLMOIFXVOEGPU-UHFFFAOYSA-N
Formula: C3F6S3
SMILES: FC(F)(F)SC(=S)SC(F)(F)F
Mol. weight [g/mol]: 246.22
CAS: 461-08-5

Physical Properties

Property code	Value	Unit	Source
gf	-1005.50	kJ/mol	Joback Method
hf	-1069.17	kJ/mol	Joback Method
hfus	20.04	kJ/mol	Joback Method
hvap	35.14	kJ/mol	Joback Method
ie	9.25	eV	NIST Webbook
log10ws	-4.51		Crippen Method
logp	3.777		Crippen Method
mcvol	108.500	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
tb	464.80	K	Joback Method
tc	672.93	K	Joback Method
tf	235.02	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.67	J/mol×K	464.80	Joback Method
cpg	226.51	J/mol×K	499.49	Joback Method
cpg	232.54	J/mol×K	534.18	Joback Method
cpg	237.84	J/mol×K	568.87	Joback Method
cpg	242.46	J/mol×K	603.55	Joback Method
cpg	246.47	J/mol×K	638.24	Joback Method

cpg	249.94	J/mol×K	672.93	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=C461085&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