Sulfur, pentafluoro(trifluoromethyl)-, (OC-6-21)-

Other names: Sulfur, pentafluoro(trifluoromethyl)-
Pentafluoro(trifluoromethyl)sulfur
CF3SF5
Trifluoromethylsulfur pentafluoride

Inchi: InChI=1S/CF8S/c2-1(3,4)10(5,6,7,8)9

InchiKey: QIYZKVMAFMDRTP-UHFFFAOYSA-N

Formula: CF8S

SMILES: FC(F)(F)S(F)(F)(F)(F)F

Mol. weight [g/mol]: 196.06

CAS: 373-80-8

Physical Properties

Property code	Value	Unit	Source
basg	640.00 ± 10.00	kJ/mol	NIST Webbook
gf	-1774.50	kJ/mol	Joback Method
hf	-1822.97	kJ/mol	Joback Method
hfus	12.97	kJ/mol	Joback Method
hvap	17.39	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.805		Crippen Method
mcvol	64.060	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	284.79	K	Joback Method
tc	421.22	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	134.80	J/mol×K	284.79	Joback Method
cpg	137.71	J/mol×K	307.53	Joback Method
cpg	140.84	J/mol×K	330.27	Joback Method
cpg	144.18	J/mol×K	353.01	Joback Method
cpg	147.69	J/mol×K	375.74	Joback Method

cpg	151.35	J/mol×K	398.48	Joback Method
cpg	155.15	J/mol×K	421.22	Joback Method
hvapt	20.20	kJ/mol	237.50	NIST Webbook
hvapt	23.80	kJ/mol	233.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C373808&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

Legend

basg: Gas basicity
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
hvapt: Enthalpy of vaporization at a given temperature
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