Cyclic octaatomic sulfur

Other names:	Cyclooctasulphur
	Octasulfur
	Octathiocane
	Orthorhombic sulfur
	S8
	Sulfur
	Sulfur (S8)
	Sulfur molecule (S8)
	Sulfur octamer
	Sulfur, mol. (S8)
	cyclooctasulfur
	sulfur, octatomic
Inchi:	InChI=1S/S8/c1-2-4-6-8-7-5-3-1
InchiKey:	JLQNHALFVCURHW-UHFFFAOYSA-N
Formula:	S8
SMILES:	S1SSSSSSS1
Mol. weight [g/mol]:	256.52
CAS:	10544-50-0

Physical Properties

Property code	Value	Unit	Source
ea	3.59 ± 0.05	eV	NIST Webbook
gf	275.96	kJ/mol	Joback Method
hf	381.09	kJ/mol	Joback Method
hfus	11.58	kJ/mol	Joback Method
hvap	63.17	kJ/mol	Joback Method
ie	9.04 ± 0.03	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	7.30 ± 0.30	eV	NIST Webbook
ie	9.60 ± 0.20	eV	NIST Webbook
ie	9.30 ± 0.20	eV	NIST Webbook
log10ws	-6.71		Crippen Method
logp	5.186		Crippen Method
mcvol	130.800	ml/mol	McGowan Method
pc	10454.96	kPa	Joback Method
rinpol	342.96		NIST Webbook

rinpol	2055.00		NIST Webbook
rinpol	2004.00		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	342.96		NIST Webbook
rinpol	2083.20		NIST Webbook
rinpol	1998.00		NIST Webbook
tb	614.80	K	Joback Method
tc	1027.34	K	Joback Method
tf	761.94	K	Joback Method
vc	0.322	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.05	J/mol×K	614.80	Joback Method
cpg	198.25	J/mol×K	683.56	Joback Method
cpg	202.57	J/mol×K	752.31	Joback Method
cpg	206.08	J/mol×K	821.07	Joback Method
cpg	208.85	J/mol×K	889.83	Joback Method
cpg	210.97	J/mol×K	958.59	Joback Method
cpg	212.49	J/mol×K	1027.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10544500&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of elemental sulfur in pure organic solvents and organic solvent-ionic liquid mixtures from 293.15 to 333.15 K:	https://www.doi.org/10.1016/j.fluid.2011.09.012
Measurement and Correlation of the Solubilities of Sulfur S8 in 10 Solvents:	https://www.doi.org/10.1021/acs.jced.7b00699
Solubility of Elemental Sulfur in Toluene between (267.15 and 313.15) K under Atmospheric Pressure:	https://www.doi.org/10.1021/je9002256
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity

ea:	Electron affinity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume