Sulfur, mol. (S8)

Other names:	Cyclooctasulphur
	Octasulfur
	Octathiocane
	Orthorhombic sulfur
	S8
	Sulfur
	Sulfur (S8)
	Sulfur molecule (S8)
	Sulfur octamer
	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]:	256.54

Physical Properties

Property code	Value	Unit	Source
ea	3.59 ± 0.05	eV	NIST Webbook
hfus	11.58	kJ/mol	Joback Method
ie	9.30 ± 0.20	eV	NIST Webbook
ie	9.04 ± 0.03	eV	NIST Webbook
ie	9.60 ± 0.20	eV	NIST Webbook
ie	7.30 ± 0.30	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
logp	5.186		Crippen Method
mcvol	130.800	ml/mol	McGowan Method
rinpol	2083.20		NIST Webbook
rinpol	2055.00		NIST Webbook
rinpol	342.96		NIST Webbook
rinpol	1998.00		NIST Webbook
rinpol	342.96		NIST Webbook
rinpol	2004.00		NIST Webbook
rinpol	1998.00		NIST Webbook

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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Measurement and Correlation of the Solubilities of Sulfur S8 in 10 Solvents:	https://www.doi.org/10.1021/acs.jced.7b00699
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10544500&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	
Solubility of elemental sulfur in pure organic solvents and organic solvent-ionic liquid mixtures from 298.15 to 338.15 K:	https://www.doi.org/10.1016/j.fluid.2011.09.012
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices