

Cyclic hexatomic sulfur

Other names:	Cyclohexasulfide
	Sulfur
	Cyclic hexatomic sulfur
	Sulfur, S6
	Sulfur hexamer
	Cyclohexasulfur
Inchi:	InChI=1S/S6/c1-2-4-6-5-3-1
InchiKey:	FEXCMMPPRBSCRG-UHFFFAOYSA-N
Formula:	S6
SMILES:	S1SSSSS1
Mol. weight [g/mol]:	192.40

Physical Properties

Property code	Value	Unit	Source
ea	3.21 ± 0.07	eV	NIST Webbook
hfus	8.46	kJ/mol	Joback Method
ie	9.20 ± 0.20	eV	NIST Webbook
ie	9.00 ± 0.03	eV	NIST Webbook
ie	9.70 ± 0.30	eV	NIST Webbook
ie	8.50 ± 0.30	eV	NIST Webbook
logp	3.889		Crippen Method
mcvol	98.100	ml/mol	McGowan Method
rinpol	1499.20		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.19	J/mol×K	510.60	Joback Method
cpg	140.00	J/mol×K	568.56	Joback Method
cpg	143.21	J/mol×K	626.51	Joback Method
cpg	145.91	J/mol×K	684.47	Joback Method
cpg	148.19	J/mol×K	742.42	Joback Method
cpg	150.15	J/mol×K	800.38	Joback Method
cpg	151.88	J/mol×K	858.34	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13798237&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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