Sulfur dimer

Other names: sulfur (S2)
sulfur molecule (S2)
sulfur, diatomic
Inchi: InChI=1S/S2/c1-2
InchiKey: MAHNFPMIPQKPPI-UHFFFAOYSA-N
Formula: S2
SMILES: S=S
Mol. weight [g/mol]: 64.13
CAS: 23550-45-0

Physical Properties

Property code	Value	Unit	Source
ea	1.56 ± 0.05	eV	NIST Webbook
ea	0.86 ± 0.10	eV	NIST Webbook
ea	2.50 ± 0.80	eV	NIST Webbook
ea	1.67 ± 0.01	eV	NIST Webbook
ea	1.66 ± 0.04	eV	NIST Webbook
gf	120.12	kJ/mol	Joback Method
hf	128.60 ± 0.30	kJ/mol	NIST Webbook
hfus	7.38	kJ/mol	Joback Method
hvap	28.93	kJ/mol	Joback Method
ie	9.56	eV	NIST Webbook
ie	9.36 ± 0.00	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.36 ± 0.00	eV	NIST Webbook
ie	9.60 ± 0.20	eV	NIST Webbook
ie	9.50 ± 0.20	eV	NIST Webbook
ie	9.50 ± 0.30	eV	NIST Webbook
ie	9.38 ± 0.03	eV	NIST Webbook
ie	9.36 ± 0.02	eV	NIST Webbook
ie	9.80 ± 0.30	eV	NIST Webbook
ie	10.10 ± 0.30	eV	NIST Webbook
ie	9.40 ± 0.10	eV	NIST Webbook
ie	9.38 ± 0.01	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.80 ± 0.50	eV	NIST Webbook
ie	9.42 ± 0.10	eV	NIST Webbook

ie	9.40 ± 0.05	eV	NIST Webbook
ie	9.32	eV	NIST Webbook
ie	9.36 ± 0.02	eV	NIST Webbook
ie	9.55	eV	NIST Webbook
log10ws	1.43		Crippen Method
logp	-0.005		Crippen Method
mcvol	39.260	ml/mol	McGowan Method
pc	8324.90	kPa	Joback Method
sgb	228.17 ± 0.01	J/mol×K	NIST Webbook
tb	335.56	K	Joback Method
tc	553.36	K	Joback Method
tf	191.30	K	Joback Method
vc	0.126	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	38.70	J/mol×K	335.56	Joback Method
cpg	39.99	J/mol×K	371.86	Joback Method
cpg	40.91	J/mol×K	408.16	Joback Method
cpg	41.50	J/mol×K	444.46	Joback Method
cpg	41.80	J/mol×K	480.76	Joback Method
cpg	41.86	J/mol×K	517.06	Joback Method
cpg	41.71	J/mol×K	553.36	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Gibbs free energy of formation of rhodium sulfides:	https://www.doi.org/10.1016/j.jct.2013.10.011
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=C23550450&Units=SI

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
sgb:	Molar entropy at standard conditions (1 bar)
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume