Mercapto radical

Inchi: InChI=1S/HS/h1H
InchiKey: PXQLVRUNWNTZOS-UHFFFAOYSA-N
Formula: HS
SMILES: [SH]
Mol. weight [g/mol]: 33.07
CAS: 13940-21-1

Physical Properties

Property code	Value	Unit	Source
ea	2.32	eV	NIST Webbook
ea	2.30 ± 0.04	eV	NIST Webbook
ea	2.31	eV	NIST Webbook
ea	2.32 ± 0.00	eV	NIST Webbook
ea	2.33 ± 0.09	eV	NIST Webbook
ea	2.32	eV	NIST Webbook
ea	2.31 ± 0.00	eV	NIST Webbook
ea	2.30 ± 0.00	eV	NIST Webbook
ea	2.32 ± 0.01	eV	NIST Webbook
ea	2.19	eV	NIST Webbook
gf	30.89	kJ/mol	Joback Method
hf	50.96	kJ/mol	Joback Method
hfpi	1143.00 ± 4.00	kJ/mol	NIST Webbook
hfpiz	1143.00 ± 4.00	kJ/mol	NIST Webbook
hfus	1.48	kJ/mol	Joback Method
hvap	22.18	kJ/mol	Joback Method
ie	10.43	eV	NIST Webbook
ie	10.37 ± 0.01	eV	NIST Webbook
ie	10.41 ± 0.03	eV	NIST Webbook
ie	10.50 ± 0.10	eV	NIST Webbook
ie	10.42 ± 0.00	eV	NIST Webbook
ie	10.42	eV	NIST Webbook
ie	10.42 ± 0.00	eV	NIST Webbook
ie	10.40 ± 0.01	eV	NIST Webbook
log10ws	-0.34		Crippen Method
logp	0.381		Crippen Method
mcvol	25.060	ml/mol	McGowan Method
pc	8116.22	kPa	Joback Method

tb	261.56	K	Joback Method
tc	445.60	K	Joback Method
tf	142.59	K	Joback Method
vc	0.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	20.22	J/mol×K	261.56	Joback Method
cpg	21.57	J/mol×K	292.23	Joback Method
cpg	22.69	J/mol×K	322.91	Joback Method
cpg	23.62	J/mol×K	353.58	Joback Method
cpg	24.36	J/mol×K	384.25	Joback Method
cpg	24.95	J/mol×K	414.93	Joback Method
cpg	25.38	J/mol×K	445.60	Joback Method

Sources

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=C13940211&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
ea: Electron affinity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfpi: Enthalpy of formation of positive ion at standard conditions
hfpiz: Enthalpy of formation of positive ion at 0K
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume