Carbonyl sulfide

Other names:	CARBON OXIDE SULFIDE
	CARBON OXYSULFIDE
	COS
	Carbon oxide sulphide
	OXYCARBON SULFIDE
	UN 2204
	carbonyl sulphide
Inchi:	InChI=1S/COS/c2-1-3
InchiKey:	JJWKPURADFRFRB-UHFFFAOYSA-N
Formula:	COS
SMILES:	O=C=S
Mol. weight [g/mol]:	60.08
CAS:	463-58-1

Physical Properties

Property code	Value	Unit	Source
af	0.1050		KDB
affp	628.50	kJ/mol	NIST Webbook
basg	602.60	kJ/mol	NIST Webbook
dm	0.70	debye	KDB
ea	0.40	eV	NIST Webbook
ea	0.46 ± 0.20	eV	NIST Webbook
gf	-165.80	kJ/mol	KDB
hf	-138.50	kJ/mol	KDB
hf	-139.00 ± 1.00	kJ/mol	NIST Webbook
hf	-139.00 ± 1.00	kJ/mol	NIST Webbook
hfpi	937.00	kJ/mol	NIST Webbook
hfpiz	937.00	kJ/mol	NIST Webbook
hfus	11.59	kJ/mol	Joback Method
hvap	30.69	kJ/mol	Joback Method
ie	11.23 ± 0.01	eV	NIST Webbook
ie	11.22 ± 0.01	eV	NIST Webbook
ie	11.19 ± 0.01	eV	NIST Webbook
ie	11.18 ± 0.01	eV	NIST Webbook
ie	11.22	eV	NIST Webbook
ie	11.19	eV	NIST Webbook
ie	11.30	eV	NIST Webbook

ie	11.18 ± 0.01	eV	NIST Webbook
ie	11.22	eV	NIST Webbook
ie	11.19	eV	NIST Webbook
ie	11.18 ± 0.01	eV	NIST Webbook
ie	11.17 ± 0.00	eV	NIST Webbook
ie	11.18 ± 0.01	eV	NIST Webbook
ie	11.19 ± 0.05	eV	NIST Webbook
ie	11.18 ± 0.00	eV	NIST Webbook
ie	11.17 ± 0.00	eV	NIST Webbook
ie	11.00 ± 1.00	eV	NIST Webbook
ie	11.19 ± 0.00	eV	NIST Webbook
ie	11.23 ± 0.01	eV	NIST Webbook
ie	11.18 ± 0.01	eV	NIST Webbook
log10ws	-4.93		Crippen Method
logp	0.251		Crippen Method
mcvol	38.570	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=3)		KDB
nfpas	%!d(float64=1)		KDB
pc	5880.00	kPa	KDB
pc	6349.00 ± 5.00	kPa	NIST Webbook
rinpol	301.00		NIST Webbook
rinpol	305.00		NIST Webbook
rinpol	304.00		NIST Webbook
rinpol	277.00		NIST Webbook
rinpol	277.00		NIST Webbook
rinpol	303.00		NIST Webbook
ripol	680.00		NIST Webbook
ripol	680.00		NIST Webbook
sl	136.31	J/mol×K	NIST Webbook
tb	223.00	K	KDB
tc	378.80 ± 0.10	K	NIST Webbook
tc	375.00	K	KDB
tf	134.30	K	KDB
tt	134.33 ± 0.02	K	NIST Webbook
tt	134.31 ± 0.20	K	NIST Webbook
vc	0.135 ± 0.002	m3/kmol	NIST Webbook
vc	0.137	m3/kmol	KDB
zc	0.2583630		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	53.92	J/mol×K	462.27	Joback Method
cpg	48.69	J/mol×K	312.40	Joback Method
cpg	50.15	J/mol×K	342.38	Joback Method
cpg	51.38	J/mol×K	372.35	Joback Method
cpg	52.41	J/mol×K	402.32	Joback Method
cpg	53.25	J/mol×K	432.30	Joback Method
cpg	46.99	J/mol×K	282.43	Joback Method
cpl	71.25	J/mol×K	220.00	NIST Webbook
hfust	4.73	kJ/mol	134.30	NIST Webbook
hfust	4.73	kJ/mol	134.33	NIST Webbook
hvapt	20.40	kJ/mol	222.50	NIST Webbook
hvapt	18.30	kJ/mol	331.50	NIST Webbook
hvapt	19.50	kJ/mol	182.00	NIST Webbook
hvapt	19.00 ± 0.10	kJ/mol	214.00	NIST Webbook
hvapt	20.89	kJ/mol	222.90	KDB
hvapt	18.51	kJ/mol	222.91	NIST Webbook
hvapt	19.50	kJ/mol	193.00	NIST Webbook
pvap	287.13	kPa	248.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation
pvap	638.23	kPa	273.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation
pvap	282.15	kPa	248.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation

pvap	651.42	kPa	273.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation
rhol	1274.00	kg/m3	174.00	KDB
sfust	35.20	J/mol×K	134.33	NIST Webbook
srf	0.02	N/m	218.20	KDB
svapt	83.02	J/mol×K	222.91	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41200e+01
Coeff. B	-1.91842e+03
Coeff. C	-2.10860e+01
Temperature range (K), min.	159.78
Temperature range (K), max.	378.77

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Experimental study and phase equilibrium modeling of systems containing acid gas and glycol:	https://www.doi.org/10.1016/j.fluid.2011.12.025
Diffusivity and solubility of carbonyl sulfide and sulfur dioxide in 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide [emim][Tf2N]: Experimental measurement and modelling:	https://www.doi.org/10.1016/j.jct.2019.01.019
Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation:	https://www.doi.org/10.1021/je400885z
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C463581&Units=SI
The Volumetric Properties of Carbonyl Sulfide and Carbon Dioxide Mixtures from T = 322 to 350 K and p = 2.9 to 35 MPa: Application to COS Hydrolysis in Subsurface Injectate Streams:	https://www.doi.org/10.1021/acs.jced.5b01061
Experimental Solubility of Carbonyl Sulfide in Sulfolane and Gamma-Butyrolactone:	https://www.doi.org/10.1021/acs.jced.7b00428
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1856.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Carbonyl Sulfide in Aqueous Solutions of Ethylene Glycol at Temperatures from (308.15 K to 323.15) K:	https://www.doi.org/10.1021/je100624p

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility

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