Sulfur dioxide

Other names:	Fermenicide liquid
	Fermenicide powder
	Fermenticide liquid
	SO2
	SULFUROUS ACID ANHYDRIDE
	SULFUROUS ANHYDRIDE
	Schwefeldioxyd
	Siarki dwutlenek
	Sulfur dioxide (SO2)
	Sulfur oxide
	Sulfur oxide (SO2)
	Sulfur superoxide
	Sulfurous oxide
	Sulphur dioxide
	UN 1079
Inchi:	InChI=1S/O2S/c1-3-2
InchiKey:	RAHZWNYVWXNFOC-UHFFFAOYSA-N
Formula:	O2S
SMILES:	O=S=O
Mol. weight [g/mol]:	64.06
CAS:	7446-09-5

Physical Properties

Property code	Value	Unit	Source
af	0.2560		KDB
affp	672.30	kJ/mol	NIST Webbook
basg	607.00	kJ/mol	NIST Webbook
basg	622.00	kJ/mol	NIST Webbook
basg	643.30	kJ/mol	NIST Webbook
dm	1.60	debye	KDB
ea	1.05	eV	NIST Webbook
ea	1.00 ± 0.05	eV	NIST Webbook
ea	1.06 ± 0.10	eV	NIST Webbook
ea	1.14 ± 0.15	eV	NIST Webbook
ea	1.10 ± 0.04	eV	NIST Webbook
ea	1.10 ± 0.10	eV	NIST Webbook
ea	1.10 ± 0.20	eV	NIST Webbook

ea	1.11 ± 0.01	eV	NIST Webbook
ea	1.00 ± 0.10	eV	NIST Webbook
gf	-300.40	kJ/mol	KDB
gyrad	1.6740		KDB
hf	-297.10	kJ/mol	KDB
hf	-296.81 ± 0.20	kJ/mol	NIST Webbook
hfus	10.50	kJ/mol	Joback Method
hvap	33.94	kJ/mol	Joback Method
ie	12.35 ± 0.00	eV	NIST Webbook
ie	12.35 ± 0.00	eV	NIST Webbook
ie	12.50 ± 0.30	eV	NIST Webbook
ie	12.40 ± 0.20	eV	NIST Webbook
ie	12.30	eV	NIST Webbook
ie	12.31	eV	NIST Webbook
ie	12.30 ± 0.01	eV	NIST Webbook
ie	12.32 ± 0.01	eV	NIST Webbook
ie	12.34	eV	NIST Webbook
ie	12.34 ± 0.02	eV	NIST Webbook
ie	12.50	eV	NIST Webbook
ie	12.54	eV	NIST Webbook
ie	12.50	eV	NIST Webbook
ie	12.50 ± 0.10	eV	NIST Webbook
log10ws	0.46		Crippen Method
logp	-0.670		Crippen Method
mcvol	34.650	ml/mol	McGowan Method
nfpah	%!d(float64=2)		KDB
pc	7884.00	kPa	KDB
pt	1.67	kPa	KDB
pt	1.67 ± 0.01	kPa	NIST Webbook
ripol	856.00		NIST Webbook
ripol	856.00		NIST Webbook
ripol	882.00		NIST Webbook
sgb	248.22 ± 0.05	J/mol×K	NIST Webbook
tb	263.10	K	KDB
tc	430.80	K	KDB
tc	430.34 ± 0.40	K	NIST Webbook
tf	197.60	K	KDB
tf	200.75 ± 0.50	K	NIST Webbook
tt	197.64 ± 0.05	K	NIST Webbook
tt	197.68	K	KDB
vc	0.122	m3/kmol	KDB
zc	0.2685310		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	49.58	J/mol×K	395.50	Joback Method
cpg	40.24	J/mol×K	270.73	Joback Method
cpg	42.58	J/mol×K	295.69	Joback Method
cpg	44.67	J/mol×K	320.64	Joback Method
cpg	46.52	J/mol×K	345.59	Joback Method
cpg	48.16	J/mol×K	370.55	Joback Method
cpg	37.64	J/mol×K	245.78	Joback Method
hvapt	24.90	kJ/mol	263.00	NIST Webbook
hvapt	24.90	kJ/mol	231.50	NIST Webbook
pvap	1479.00	kPa	343.15	Thermodynamic study of binary systems containing sulfur dioxide: measurements and molecular modelling
pvap	1469.00	kPa	343.15	Thermodynamic study of binary systems containing sulfur dioxide: measurements and molecular modelling
pvap	2883.00	kPa	373.15	Thermodynamic study of binary systems containing sulfur dioxide: measurements and molecular modelling
pvap	5836.00	kPa	413.15	Thermodynamic study of binary systems containing sulfur dioxide: measurements and molecular modelling
pvap	5978.00	kPa	413.15	Thermodynamic study of binary systems containing sulfur dioxide: measurements and molecular modelling

rhol	1455.00	kg/m3	263.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48701e+01
Coeff. B	-2.33358e+03
Coeff. C	-3.55000e+01
Temperature range (K), min.	197.67
Temperature range (K), max.	430.75

Sources

Investigation of SO2 solubilities in some biobased solvents and their thermodynamic properties:	https://www.doi.org/10.1016/j.jct.2017.12.021
Experimental determination of dissociation constant, Henry's constant, heat of reactions, SO2 absorbed and gas bubble liquid interfacial area for dilute sulphur dioxide absorption into water:	https://www.doi.org/10.1016/j.fluid.2007.01.015
Solubility for dilute sulfur dioxide in binary mixtures of N,N-dimethylformamide + ethylene glycol at 298.15 K and 122.66 kPa:	https://www.doi.org/10.1016/j.jct.2013.02.010
New experimental density data and derived thermophysical properties of carbon dioxide - Sulphur dioxide binary mixture (CO2 - SO2) in gas, liquid and supercritical phases from 273 K to 353 K and at pressures up to 42 MPa:	https://www.doi.org/10.1016/j.fluid.2017.09.014
Absorption, desorption and spectroscopic investigation of sulfur dioxide in the binary system ethylene glycol + dimethyl sulfoxide:	https://www.doi.org/10.1016/j.fluid.2015.06.047
Solubility Properties and Spectral Characterization of Dilute SO2 in Binary Mixtures of Urea + Ethylene Glycol:	https://www.doi.org/10.1021/je5009119
Solubility of dilute sulfur dioxide in binary mixtures of ethylene glycol and tetraethylene glycol dimethyl ether:	https://www.doi.org/10.1016/j.fluid.2015.03.002
Solubility Properties and Absorption Mechanism Investigation of Dilute SO2 in Propylene Glycol Monomethyl Ether + Dimethyl Sulfoxide System:	https://www.doi.org/10.1021/acs.jced.6b00660
Thermodynamic study of binary systems containing sulfur dioxide: measurements and molecular modeling:	https://www.doi.org/10.1016/j.fluid.2011.02.008
Thermodynamic Study of binary an ternary systems containing CO2 + impurities in the context of CO2 transportation:	https://www.doi.org/10.1016/j.fluid.2014.08.031
Thermodynamic properties and spectral investigation of dilute sulfur dioxide in binary system N,N-dimethylformamide + diethylene glycol:	https://www.doi.org/10.1016/j.fluid.2015.01.019
Experimental study and thermodynamical modelling of solubilities of SO2, H2S and CO2in N-dodecylimidazole and 1,1-[oxybis(2,1-ethanediyloxy-2,1-ethanediyl)]bis(imidazole): An evaluation of their potential application in the separation of acidic gases:	https://www.doi.org/10.1016/j.fluid.2014.06.026
SO2 Solubility in 50 wt % H2SO4 at Elevated Temperatures and Pressures:	https://www.doi.org/10.1021/je4002366
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1936
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Comparative Study of the Solubilities of SO2 in Five Low Volatile Organic Solvents (Sulfolane, Ethylene Glycol, Propylene Carbonate, N-Methylimidazole, and N-Methylpyrrolidone):	https://www.doi.org/10.1021/je4007713
Solubility and thermodynamic properties of SO2 in three low volatile urea derivatives:	https://www.doi.org/10.1016/j.jct.2016.05.004
Solubility of Dilute SO2 in the Binary System Poly Ethylene Glycol 300 + Dimethyl Sulfoxide at T = 298.15 K and p = 123.15 kPa and Mixtures' Excess Properties at T = (298.15, 303.15, 308.15, 313.15 and 318.15) K:	https://www.doi.org/10.1021/je500067f
Volumetric properties and phase behavior of sulfur dioxide, carbon disulfide and oxygen in high-pressure carbon dioxide fluid:	https://www.doi.org/10.1016/j.fluid.2018.08.012
Absorption of SO2 in different electrolyte solutions, seawater and brine:	https://www.doi.org/10.1016/j.fluid.2015.05.041
Thermodynamic study of binary systems containing sulphur dioxide and nitric oxide: Measurements and modelling:	https://www.doi.org/10.1016/j.fluid.2017.12.036
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7446095&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Diffusivity and solubility of carbonyl sulfide and sulfur dioxide in 1-ethyl-3-methylimidazolium bis (trifluoromethyl) sulfonylimide ([emim][Tf2N]): Experimental measurement and modelling.	https://www.doi.org/10.1016/j.jct.2019.01.019
Crippen Method	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic investigation of room temperature ionic liquid: The heat capacity and standard enthalpy of formation of EMIES:	https://www.doi.org/10.1016/j.tca.2006.04.022
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Solubilities and thermodynamic properties of SO2 in five biobased solvents:	https://www.doi.org/10.1016/j.jct.2015.09.017
Gas Liquid Equilibrium Data for a Mixture Gas of Sulfur Dioxide + Nitrogen with Ethylene Glycol Aqueous Solutions at 298.15 K and 1.013 kPa.	https://www.doi.org/10.1021/je800271e
Solubility of SO2 in Caprolactam Tetrabutyl Ammonium Bromide Ionic Liquids:	https://www.doi.org/10.1021/je900565e
Density and Spectral Studies for SO2 in Binary System of Tri-ethylene Glycol + Dimethyl Sulfoxide at T = 298.15, 303.15, and 308.15 K and p = 129.19 kPa:	https://www.doi.org/10.1021/acs.jced.5b00981
Gas Liquid Equilibrium Data for the Mixture Gas of Sulfur Dioxide/Nitrogen Solubility for dilute sulfur dioxide aqueous solutions at 298.15 K under Low Pressures:	https://www.doi.org/10.1021/je800117x
Gas Liquid Equilibrium Data for the Mixture Gas of Sulfur Dioxide/Nitrogen at 303.15 and 308.15 K and p = 129.19 kPa: Ethylene Glycol at Temperatures from 298.15 to 313.15 K under Low Pressures:	https://www.doi.org/10.1016/j.fluid.2014.04.019
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Viscosities, excess properties, and thermodynamics of binary system N, N-dimethylformamide + diethylene glycol:	

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
dm:	Dipole Moment
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pt:	Triple Point Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
ripol:	Polar retention indices
sgb:	Molar entropy at standard conditions (1 bar)
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter