Carbon disulfide

Other names:	Alcohol of sulfur
	CARBON BISULFIDE
	CS2
	Carbon bisulfuret
	Carbon bisulphide
	Carbon sulfide
	Carbon sulfide (CS2)
	Carbon sulphide
	Carbon-disulphide-
	DITHIOCARBONIC ANHYDRIDE
	Kohlendisulfid
	Koolstofdisulfide
	Methyl disulfide
	NCI-C04591
	Rcra waste number P022
	Schwefelkohlenstoff
	Solfuro di carbonio
	Sulfocarbonic anhydride
	Sulphocarbonic anhydride
	UN 1131
	Weeviltox
	Wegla dwusiarczek
	carbon disulphide
Inchi:	InChI=1S/CS2/c2-1-3
InchiKey:	QGJOPFRUJISHPQ-UHFFFAOYSA-N
Formula:	CS2
SMILES:	S=C=S
Mol. weight [g/mol]:	76.14
CAS:	75-15-0

Physical Properties

Property code	Value	Unit	Source
af	0.1090		KDB
affp	681.90	kJ/mol	NIST Webbook
aigt	373.15	K	KDB
basg	657.70	kJ/mol	NIST Webbook

chg	-1112.00	kJ/mol	NIST Webbook
chl	-1687.20 ± 0.50	kJ/mol	NIST Webbook
dm	0.00	debye	KDB
ea	1.00 ± 0.20	eV	NIST Webbook
ea	0.94 ± 0.32	eV	NIST Webbook
ea	0.50 ± 0.20	eV	NIST Webbook
ea	0.60 ± 0.10	eV	NIST Webbook
ea	6.94e-04	eV	NIST Webbook
ea	0.80	eV	NIST Webbook
ea	0.51 ± 0.10	eV	NIST Webbook
ea	0.58 ± 0.05	eV	NIST Webbook
ea	0.55 ± 0.00	eV	NIST Webbook
ea	1.46 ± 0.02	eV	NIST Webbook
ea	0.89 ± 0.20	eV	NIST Webbook
fll	1.30	% in Air	KDB
flu	50.00	% in Air	KDB
fpo	243.15	K	KDB
gf	66.95	kJ/mol	KDB
gyrad	1.4240		KDB
hf	117.10	kJ/mol	KDB
hf	117.10 ± 0.79	kJ/mol	NIST Webbook
hfl	89.41 ± 0.71	kJ/mol	NIST Webbook
hfus	12.10	kJ/mol	Joback Method
hvap	31.60	kJ/mol	Joback Method
ie	10.08 ± 0.00	eV	NIST Webbook
ie	10.06	eV	NIST Webbook
ie	10.00 ± 1.00	eV	NIST Webbook
ie	10.07 ± 0.00	eV	NIST Webbook
ie	10.05 ± 0.08	eV	NIST Webbook
ie	10.06 ± 0.03	eV	NIST Webbook
ie	10.07	eV	NIST Webbook
ie	10.12	eV	NIST Webbook
ie	10.08	eV	NIST Webbook
ie	10.08	eV	NIST Webbook
ie	10.07 ± 0.01	eV	NIST Webbook
ie	10.10 ± 0.10	eV	NIST Webbook
ie	10.06	eV	NIST Webbook
ie	10.06 ± 0.01	eV	NIST Webbook
ie	10.06	eV	NIST Webbook
ie	10.07 ± 0.10	eV	NIST Webbook
ie	10.07 ± 0.01	eV	NIST Webbook
ie	10.12 ± 0.01	eV	NIST Webbook
ie	10.13	eV	NIST Webbook
ie	10.07	eV	NIST Webbook

ie	10.08 ± 0.01	eV	NIST Webbook
ie	10.14 ± 0.01	eV	NIST Webbook
ie	10.06 ± 0.01	eV	NIST Webbook
ie	10.11 ± 0.01	eV	NIST Webbook
ie	10.08	eV	NIST Webbook
ie	10.08 ± 0.00	eV	NIST Webbook
ie	10.08	eV	NIST Webbook
ie	10.13	eV	NIST Webbook
ie	10.09	eV	NIST Webbook
ie	10.08	eV	NIST Webbook
ie	10.07 ± 0.01	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.13	eV	NIST Webbook
ie	10.08 ± 0.01	eV	NIST Webbook
log10ws	-1.37		Crippen Method
logp	1.018		Crippen Method
mcvol	49.050	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=2)		KDB
pc	7900.00	kPa	KDB
rinpol	514.00		NIST Webbook
rinpol	533.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	537.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	568.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	539.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	564.40		NIST Webbook
rinpol	576.00		NIST Webbook
rinpol	558.00		NIST Webbook
rinpol	557.30		NIST Webbook
rinpol	539.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	544.00		NIST Webbook
rinpol	538.00		NIST Webbook
rinpol	568.00		NIST Webbook
rinpol	564.00		NIST Webbook
rinpol	558.00		NIST Webbook
rinpol	557.00		NIST Webbook
rinpol	517.00		NIST Webbook

rinpol	536.00		NIST Webbook
rinpol	530.00		NIST Webbook
rinpol	537.00		NIST Webbook
rinpol	537.00		NIST Webbook
rinpol	533.00		NIST Webbook
rinpol	536.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	512.00		NIST Webbook
rinpol	540.00		NIST Webbook
rinpol	569.00		NIST Webbook
rinpol	568.00		NIST Webbook
rinpol	544.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	534.00		NIST Webbook
rinpol	534.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	549.00		NIST Webbook
rinpol	537.00		NIST Webbook
rinpol	536.00		NIST Webbook
rinpol	561.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	518.00		NIST Webbook
rinpol	524.00		NIST Webbook
rinpol	513.00		NIST Webbook
rinpol	512.00		NIST Webbook
ripol	745.00		NIST Webbook
ripol	733.00		NIST Webbook
ripol	745.00		NIST Webbook
ripol	701.00		NIST Webbook
ripol	701.00		NIST Webbook
ripol	751.00		NIST Webbook
ripol	780.00		NIST Webbook
ripol	710.00		NIST Webbook
ripol	748.00		NIST Webbook
ripol	745.00		NIST Webbook
ripol	748.00		NIST Webbook
ripol	701.00		NIST Webbook
ripol	735.00		NIST Webbook
sl	151.00	J/mol×K	NIST Webbook
tb	319.00	K	KDB
tc	552.00	K	KDB
tc	552.00	K	NIST Webbook

tf	161.00 ± 2.00	K	NIST Webbook
tf	161.60 ± 1.50	K	NIST Webbook
tf	161.60	K	KDB
tf	161.55 ± 0.40	K	NIST Webbook
tf	161.35 ± 0.20	K	NIST Webbook
tf	161.00 ± 2.00	K	NIST Webbook
tf	161.60 ± 0.40	K	NIST Webbook
tf	162.30 ± 0.50	K	NIST Webbook
tf	156.35 ± 0.40	K	NIST Webbook
tt	161.11 ± 0.02	K	NIST Webbook
tt	161.59 ± 0.20	K	NIST Webbook
vc	0.173	m3/kmol	KDB
zc	0.2977810		KDB
zra	0.28		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	60.72	J/mol×K	555.42	Joback Method
cpg	57.76	J/mol×K	361.71	Joback Method
cpg	58.82	J/mol×K	400.45	Joback Method
cpg	59.60	J/mol×K	439.19	Joback Method
cpg	60.16	J/mol×K	477.93	Joback Method
cpg	60.52	J/mol×K	516.67	Joback Method
cpg	60.79	J/mol×K	594.16	Joback Method
cpl	76.02	J/mol×K	297.43	NIST Webbook
cpl	78.99	J/mol×K	298.00	NIST Webbook
cpl	74.89	J/mol×K	294.81	NIST Webbook
cpl	77.80	J/mol×K	293.00	NIST Webbook
cpl	76.10	J/mol×K	301.20	NIST Webbook
hfust	4.39	kJ/mol	161.10	NIST Webbook
hfust	4.39	kJ/mol	161.11	NIST Webbook
hvapt	27.60	kJ/mol	330.50	NIST Webbook
hvapt	26.74	kJ/mol	319.00	KDB
hvapt	26.74	kJ/mol	319.40	NIST Webbook
hvapt	28.70	kJ/mol	304.50	NIST Webbook
hvapt	27.10	kJ/mol	453.00	NIST Webbook
hvapt	28.50	kJ/mol	306.50	NIST Webbook
hvapt	27.40	kJ/mol	373.00	NIST Webbook
hvapt	27.00	kJ/mol	442.50	NIST Webbook
hvapt	28.70	kJ/mol	511.50	NIST Webbook

hvapt	28.70	kJ/mol	286.50	NIST Webbook
hvapt	28.10	kJ/mol	315.00	NIST Webbook
hvapt	28.10 ± 0.10	kJ/mol	282.00	NIST Webbook
hvapt	26.70 ± 0.10	kJ/mol	319.00	NIST Webbook
pvap	17.30	kPa	273.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation
pvap	17.00	kPa	273.08	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)
pvap	49.00	kPa	298.40	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)

pvap	116.00	kPa	323.50	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)
pvap	240.00	kPa	348.45	Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan)
pvap	4.50	kPa	248.15	Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled with the Wilson Equation
rhol	1293.00	kg/m3	273.00	KDB
sfust	27.24	J/mol×K	161.11	NIST Webbook
srf	0.03	N/m	293.20	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46236e+01
Coeff. B	-3.00601e+03

Coeff. C	-1.87560e+01
Temperature range (K), min.	228.44
Temperature range (K), max.	512.00

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.61912e+01
Coeff. B	-4.56318e+03
Coeff. C	-4.81722e+00
Coeff. D	4.82906e-06
Temperature range (K), min.	161.58
Temperature range (K), max.	552.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Pure (Korean Thermophysical Properties Databank):	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1812
Experimental solubility data of various n-alkane waxes: effects of alkane chain length, alkane odd versus even carbon number, structures, and solvent:	https://www.doi.org/10.1016/j.fluid.2004.10.021
Volumetric properties and phase behavior of sulfur dioxide/carbon dioxide and oxygen/carbon dioxide fluid:	https://www.doi.org/10.1016/j.fluid.2018.08.012
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75150&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Determination of Henry's Law Constants Using Internal Standards With Benchmark Values:	https://www.doi.org/10.1021/je3010535
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1812
Vapor Liquid Equilibrium for Several Compounds Relevant to the Biofuels Industry Modeled With the Wilson Equation:	https://www.doi.org/10.1021/je400885z
High Pressure Phase Behavior of Carbon Dioxide in Carbon Disulfide and Carbon Tetrachloride:	https://www.doi.org/10.1021/je101225a
Measurement of VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmercaptan or ethylmercaptan):	https://www.doi.org/10.1016/j.fluid.2007.07.013
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1812

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature

basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
ea:	Electron affinity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpo:	Flash Point (Open Cup Method)
gf:	Standard Gibbs free energy of formation
gyrad:	Radius of Gyration
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
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
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
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.