Hydrogen sulfide

Other names: Acide sulfhydrique

DIHYDROGEN MONOSULFIDE

Dihydrogen sulfide

H2S

HYDROSULFURIC ACID

Hepatic acid Hepatic gas

Hydrogen monosulfide Hydrogen sulfide (H2S) Hydrogen sulphide Hydrogene sulfure Idrogeno solforato

Rcra waste number U135

SULFUR HYDRIDE Schwefelwasserstoff

Sewer gas Siarkowodor Stink damp

Sulfureted hydrogen Sulfuretted hydrogen

UN 1053

Zwavelwaterstof

Inchi: InChi=1S/H2S/h1H2

InchiKey: RWSOTUBLDIXVET-UHFFFAOYSA-N

 Formula:
 H2S

 SMILES:
 S

 Mol. weight [g/mol]:
 34.08

 CAS:
 7783-06-4

Physical Properties

Property code	Value	Unit	Source
af	0.0810		KDB
affp	705.00	kJ/mol	NIST Webbook
basg	673.80	kJ/mol	NIST Webbook
dm	0.90	debye	KDB
gf	-33.08	kJ/mol	KDB

gyrad	0.6040		KDB
hf	20.18	kJ/mol	KDB
hf	-20.60 ± 0.50	kJ/mol	NIST Webbook
ie	10.45 ± 0.01	eV	NIST Webbook
ie	10.43	eV	NIST Webbook
ie	10.43	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
ie	10.47 ± 0.01	eV	NIST Webbook
ie	10.47	eV	NIST Webbook
ie	10.45	eV	NIST Webbook
ie	10.43	eV	NIST Webbook
ie	10.46 ± 0.01	eV	NIST Webbook
ie	10.45 ± 0.03	eV	NIST Webbook
ie	20.12	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
ie	12.76	eV	NIST Webbook
ie	10.47	eV	NIST Webbook
ie	10.56 ± 0.05	eV	NIST Webbook
ie	18.00	eV	NIST Webbook
ie	14.82	eV	NIST Webbook
ie	10.48	eV	NIST Webbook
ie	12.62	eV	NIST Webbook
ie	10.47 ± 0.00	eV	NIST Webbook
ie	14.91	eV	NIST Webbook
ie	10.48	eV	NIST Webbook
ie	10.00 ± 4.00	eV	NIST Webbook
ie	10.45 ± 0.01	eV	NIST Webbook
ie	10.46 ± 0.00	eV	NIST Webbook
ie	10.42	eV	NIST Webbook
ie	10.43 ± 0.01	eV	NIST Webbook
ie	12.81	eV	NIST Webbook
ie	14.79	eV	NIST Webbook
ie	10.46 ± 0.01	eV	NIST Webbook
ie	18.00	eV	NIST Webbook
ie	20.80	eV	NIST Webbook
log10ws	-0.08		Crippen Method
logp	0.113		Crippen Method
mcvol	27.210	ml/mol	McGowan Method
nfpaf	%!d(float64=4)	militio	KDB
nfpah	%!d(float64=4)		KDB
pc	8940.00	kPa	KDB
pc pc	8970.00 ± 18.00	kPa kPa	NIST Webbook
	8962.91 ± 30.00	kPa kPa	NIST Webbook
pc		kPa kPa	NIST Webbook
pt	23.20 ± 0.50	KPa	INIO I VVEDDOOK

pt	23.18	kPa	KDB
rhoc	347.63 ± 3.41	kg/m3	NIST Webbook
rinpol	340.00		NIST Webbook
rinpol	338.00		NIST Webbook
rinpol	338.00		NIST Webbook
ripol	480.00		NIST Webbook
ripol	480.00		NIST Webbook
ripol	480.00		NIST Webbook
sgb	205.81 ± 0.05	J/mol×K	NIST Webbook
tb	213.60	K	KDB
tb	212.87 ± 0.07	K	NIST Webbook
tc	373.40 ± 0.15	K	NIST Webbook
tc	373.30 ± 0.37	K	NIST Webbook
tc	373.20	K	KDB
tf	190.85 ± 1.50	K	NIST Webbook
tf	187.60	K	KDB
tt	187.66 ± 0.06	K	NIST Webbook
tt	187.67	K	KDB
tt	187.61 ± 0.03	K	NIST Webbook
VC	0.099	m3/kmol	KDB
ZC	0.2852290		KDB
zra	0.28		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
dvisc	0.0000188	Pa×s	461.92	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K
dvisc	0.0000119	Paxs	291.61	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K

dvisc	0.0000119	Paxs	292.30	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000268	Paxs	682.03	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000268	Paxs	681.36	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000258	Paxs	652.32	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000258	Paxs	652.30	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000248	Paxs	623.19	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000248	Paxs	623.07	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	

dvisc	0.0000119	Paxs	292.46	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000238	Paxs	594.02	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000238	Paxs	593.95	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000228	Paxs	565.29	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000227	Paxs	565.19	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000219	Paxs	542.61	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000219	Paxs	542.48	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	

dvisc	0.0000210	Paxs	518.75	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000210	Paxs	518.68	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000199	Paxs	490.20	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000121	Paxs	297.01	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000119	Paxs	292.77	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000188	Paxs	461.72	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000177	Paxs	433.81	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	

dvisc	0.0000177	Paxs	433.66	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000166	Paxs	405.86	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000166	Paxs	405.76	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000154	Paxs	378.19	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000154	Paxs	378.01	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000143	Paxs	350.59	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000132	Paxs	323.96	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	

dvisc	0.0000143	Paxs	350.47	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000132	Paxs	323.94	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000199	Paxs	490.09	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
dvisc	0.0000121	Paxs	296.89	Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low Density in the Temperature Range from (292 to 682) K	
hsubt	25.40	kJ/mol	175.50	NIST Webbook	
hsubt	22.50	kJ/mol	135.00	NIST Webbook	
hvapt	19.50	kJ/mol	206.50	NIST Webbook	
hvapt	21.90	kJ/mol	200.00	NIST Webbook	
hvapt	18.60	kJ/mol	295.50	NIST Webbook	
pvap	2024.00	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	
				methylmercaptan	
				or ethylmercaptan)	

pvap	384.00	kPa	243.02	Phase Equilibria of H2S-Hydrocarbons (Propane, n-Butane, and n-Pentane) Binary Systems at Low Temperatures	
pvap	167.30	kPa	222.83	Phase Equilibria of H2S-Hydrocarbons (Propane, n-Butane, and n-Pentane) Binary Systems at Low Temperatures	
pvap	1029.30	kPa	273.13	Phase Equilibria of H2S-Hydrocarbons (Propane, n-Butane, and n-Pentane) Binary Systems at Low Temperatures	
pvap	1030.20	kPa	273.12	Phase Equilibria of H2S-Hydrocarbons (Propane, n-Butane, and n-Pentane) Binary Systems at Low Temperatures	
pvap	379.40	kPa	243.20	Phase Equilibria of H2S-Hydrocarbons (Propane, n-Butane, and n-Pentane) Binary Systems at Low Temperatures	
pvap	380.20	kPa	243.18	Phase Equilibria of H2S-Hydrocarbons (Propane, n-Butane, and n-Pentane) Binary Systems at Low Temperatures	

pvap	5812.00	kPa	348.45	Measurement of	
h . Ah	55.2.00		5.0.10	VLE (TPx or TPxy data) for hydrogen sulfide + (dimethylsulfide or ethylmethylsulfide or carbon disulfide) and methane solubilities in (dimethylsulfide or ethylmethylsulfide or methylmethylsulfide or methylmercaptan or ethylmercaptan)	
pvap	1793.70	kPa	293.43	Phase Equilibria of H2S-Hydrocarbons (Propane, n-Butane, and n-Pentane) Binary Systems at Low Temperatures	
pvap	3564.00	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	1033.00	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 methylmethylsulfide or methylmercaptan or ethylmercaptan)	

pvap	8932.10	kPa	373.15	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	7533.00	kPa	363.16	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	6319.20	kPa	353.17	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	5261.20	kPa	343.16	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	4339.50	kPa	333.17	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	

pvap	3540.40	kPa	323.18	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	2847.20	kPa	313.11	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	2259.60	kPa	303.08	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	2022.20	kPa	298.41	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	1779.50	kPa	293.30	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	

pvap	1767.90	kPa	293.10	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	1566.60	kPa	288.31	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	1371.10	kPa	283.26	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	1194.10	kPa	278.24	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	1032.30	kPa	273.17	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	

pvap	885.70	kPa	268.02	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	757.70	kPa	263.00	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	644.50	kPa	258.01	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	456.70	kPa	248.01	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	380.10	kPa	243.04	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	

pvap	313.90	kPa	238.04	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	257.40	kPa	233.11	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	209.10	kPa	228.20	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	167.40	LD-		Manager Parel d	
		kPa	223.19	Vapour liquid equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to about 6.9MPa	
pvap	544.20	kPa kPa	252.97	equilibrium data for the hydrogen sulphide + n-heptane system at temperatures from 293.25 to 373.22K and pressures up to	

Correlations

Information	Value
IIIIOIIIIalioii	value

Property code	pvap		
Equation	ln(Pvp) = A + B/(T + C)		
Coeff. A	1.43785e+01		
Coeff. B	-1.84720e+03		
Coeff. C	-2.35400e+01		
Temperature range (K), min.	187.68		
Temperature range (K), max.	373.53		

Sources

P.rho.T Data for Hydrogen Sulfide + Propane from (263 to 363) K at Selybilitysof HeS4in Impic Liquids 1-Ethyl-3-methylimidazolium Aekilitroshtyshaer(EwilidgiPF6]) Agudges Southons of Therogins in the Bown Hallen (Brown) (Thick In Inches (Brown) (Thick Vapour India) equilibrium data for the hydrogen sulphide + n-heptane system Soluhiptyatures riom 293.25 to 373.22K ar(a-bustsexueshyd)ta-methytimidaaolium tonk liquids with different anions:

Phase Equilibria of H2S-Hydrocarbons (Propane, n-Butane, and n-Pentane) **Expany Bystahstudy aw Tenase**ratures:
equilibrium modeling of systems **Worksward Metaga**s and glycol:

Crippen Method:

Vapour pressure and excess Gibbs free https://www.doi.org/10.1016/j.jct.2006.03.013 energy of binary mixtures of hydrogen solubility of the hand, by the horizontal mixtures of hydrogen solubility of the hand, by the horizontal modelling of the modynamical modelling of the modynamical modelling of the modynamical modelling of the hydrogen hit mixtures of hydrogen hit ps://www.doi.org/10.1016/j.fluid.2014.06.026 the modynamical modelling of the hydrogen hit ps://www.doi.org/10.1016/j.jct.2018.10.013 in the hydrogen hit ps://www.doi.org/10.1016/j.jct.2018.10.013 in the hydrogen hit ps://www.doi.org/10.1021/acs.jced.5b00680 https://www.doi.org/10.1021/je900716q https://www.doi.org/10.1016/j.fluid.2016.04.024 preparties of the hydrogen hit ps://www.doi.org/10.1016/j.fluid.2016.04.024 preparties of the hydrogen hit ps://www. Hissan Rawie if it imizka for \$58 K and hydrogens supplied Mpnethane system ชาตุล พุทธา หาก system ชาตุล พุทธา หาก รุงรายา หา [hmim][Tf2N]:

https://www.doi.org/10.1021/je100851w https://www.doi.org/10.1021/je100794k

https://www.doi.org/10.1021/je900721q

https://www.doi.org/10.1016/j.fluid.2011.04.010

https://www.doi.org/10.1016/j.fluid.2006.09.021

https://www.doi.org/10.1016/j.fluid.2010.08.027

https://www.cheric.org/files/research/kdb/mol/mol1917.mol

https://www.doi.org/10.1021/je300111m

https://www.doi.org/10.1016/j.fluid.2011.12.025

http://link.springer.com/article/10.1007/BF02311772

https://www.chemeo.com/doc/models/crippen_log10ws

Vapour pressure and excess Gibbs free https://www.doi.org/10.1016/j.jct.2006.03.013

https://www.doi.org/10.1016/j.jct.2015.01.001

https://www.doi.org/10.1016/j.fluid.2013.07.050

https://www.doi.org/10.1016/j.jct.2012.02.009

https://www.doi.org/10.1021/acs.jced.7b01004

https://www.doi.org/10.1016/j.fluid.2017.09.003

https://www.doi.org/10.1016/j.jct.2009.04.014

H2S-loaded aqueous weeklenged with the solution:

Reference Viscosities of Gaseous Methane and Hydrogen Sulfide at Low รู๊อใหล่เป็นกลู้ก็ย่างใหลูคู่อาณีเหย็นสิ่นใช้ เพื่อ from https://www.doi.org/10.1007/s10765-007-0185-z

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absorption and religiating acceptances one solubility of https://www.doi.org/10.1016/j.fluid.2008.05.00

1-ethyl-3-methylimidazolium Studylor, the sqlubility of CO2, H2S and https://www.doi.org/10.1016/j.jct.2013.05.038

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hexafluorophosphate: Experimental Measuraments of H2S solubility in aqueous disopropanolamine solutions Experimental presentation of hydrogen sulfide solubility in aqueous sulfolane solubili

Solumenty of H2S in Aqueous
Diisopropanolamine + Piperazine
Solument | None propinite film | Data and
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Expressivated and modelling investigation of H2S solubility in Experimental and modelling study of the property of the propert

Sulfide and carbon dioxide in อักกอสกับของค์สัตพิสิตอุลดีH2S Using มีคุณทางอุญที่อักมีสิตอุลดีH2S Using มีคุณทางอุญที่อัลดีประการของค่า เมื่อสถังทุกเลืองอุปอุที่มีของ blands of sulphide in aqueous blends of N-methyldiethanolamine and 2-

aminoethyl)amino)ethanol and correlating by the Deshmukh-Mather

Measuring the density and viscosity of https://www.doi.org/10.1016/j.jct.2016.06.007

http://pubs.acs.org/doi/abs/10.1021/ci990307l

https://www.doi.org/10.1021/je200371n

https://www.doi.org/10.1016/j.jct.2015.04.032

https://www.doi.org/10.1016/j.fluid.2008.05.001

http://webbook.nist.gov/cgi/cbook.cgi?ID=C7783064&Units=SI

https://www.doi.org/10.1016/j.fluid.2012.11.009

https://www.doi.org/10.1021/acs.jced.5b00318

https://www.doi.org/10.1016/j.fluid.2007.07.013

https://www.doi.org/10.1016/j.jct.2019.02.024

https://www.doi.org/10.1021/je8009495

https://www.doi.org/10.1021/acs.jced.5b00669 https://www.doi.org/10.1016/j.jct.2019.03.031

https://www.doi.org/10.1016/j.fluid.2016.08.002

https://www.doi.org/10.1016/j.fluid.2010.01.013

https://www.doi.org/10.1016/j.jct.2019.02.022

https://www.doi.org/10.1016/j.jct.2017.11.014

https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

https://www.doi.org/10.1016/j.fluid.2014.01.020

https://www.doi.org/10.1021/je1004005

https://www.doi.org/10.1016/j.jct.2016.04.012

Leaend

af: Acentric Factor affp: Proton affinity basg: Gas basicity dm: **Dipole Moment** dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

gyrad: Radius of Gyration

hf: Enthalpy of formation at standard conditions hsubt: Enthalpy of sublimation at a given temperature **hvapt:** Enthalpy of vaporization at a given temperature

ie: Ionization energy

log10ws:Log10 of Water solubility in mol/llogp:Octanol/Water partition coefficientmcvol:McGowan's characteristic volume

nfpaf: NFPA Fire Ratingnfpah: NFPA Health Ratingpc: Critical Pressure

pt: Triple Point Pressure

pvap: Vapor pressurerhoc: Critical densityrhol: Liquid Density

rinpol: Non-polar retention indices

ripol: Polar retention indices

sgb: Molar entropy at standard conditions (1 bar)

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) pointtt: Triple Point Temperature

vc: Critical Volume

zc: Critical Compressibility
zra: Rackett Parameter

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