1-Hexyne

Other names:	BUTYLACETYLENE
	Hex-1-yne
	Hexyne
	N-BUTYLACETYLENE
	NSC 9709
Inchi:	InChI=1S/C6H10/c1-3-5-6-4-2/h1H,4-6H2,2H3
InchiKey:	CGHIBGNXEGJPQZ-UHFFFAOYSA-N
Formula:	C6H10
SMILES:	C#CCCCC
Mol. weight [g/mol]:	82.14
CAS:	693-02-7

Physical Properties

Property code	Value	Unit	Source
af	0.2490		KDB
affp	799.80	kJ/mol	NIST Webbook
basg	774.80	kJ/mol	NIST Webbook
gf	222.71	kJ/mol	Joback Method
hcg	3889.86	kJ/mol	KDB
hcn	3670.205	kJ/mol	KDB
hf	122.30 ± 1.20	kJ/mol	NIST Webbook
hfus	14.27	kJ/mol	Joback Method
hvap	28.81	kJ/mol	Joback Method
ie	10.52 ± 0.05	eV	NIST Webbook
ie	9.95 ± 0.05	eV	NIST Webbook
ie	10.03 ± 0.05	eV	NIST Webbook
ie	10.07 ± 0.01	eV	NIST Webbook
ie	10.07 ± 0.02	eV	NIST Webbook
log10ws	-2.36		Estimated Solubility Method
log10ws	-2.36		Aqueous Solubility Prediction Method
logp	1.810		Crippen Method
mcvol	86.800	ml/mol	McGowan Method
pc	3690.00	kPa	KDB
rinpol	587.00		NIST Webbook
rinpol	584.00		NIST Webbook

rinpol	587.30		NIST Webbook
rinpol	588.00		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	583.00		NIST Webbook
rinpol	590.00		NIST Webbook
rinpol	588.20		NIST Webbook
rinpol	587.30		NIST Webbook
rinpol	612.00		NIST Webbook
rinpol	586.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	586.00		NIST Webbook
rinpol	611.00		NIST Webbook
rinpol	586.00		NIST Webbook
rinpol	587.30		NIST Webbook
rinpol	584.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	587.00		NIST Webbook
rinpol	610.00		NIST Webbook
ripol	827.00		NIST Webbook
ripol	827.00		NIST Webbook
ripol	847.30		NIST Webbook
ripol	833.00		NIST Webbook
ripol	837.00		NIST Webbook
tb	344.65 ± 1.00	K	NIST Webbook
tb	344.40 ± 2.00	K	NIST Webbook
tb	343.40 ± 0.70	K	NIST Webbook
tb	343.65 ± 1.50	K	NIST Webbook
tb	344.15 ± 1.00	K	NIST Webbook
tb	344.15 ± 0.50	K	NIST Webbook
tb	323.15	K	NIST Webbook
tb	344.15 ± 1.50	K	NIST Webbook
tb	345.15 ± 1.50	K	NIST Webbook
tb	344.65 ± 1.50	K	NIST Webbook
tb	344.55 ± 0.30	K	NIST Webbook
tb	343.65 ± 1.50	K	NIST Webbook
tb	344.65 ± 1.50	K	NIST Webbook
tb	343.65 ± 1.50	K	NIST Webbook
tb	344.50 ± 0.30	K	NIST Webbook
tb	344.65 ± 0.70	K	NIST Webbook
tb	344.00 ± 2.00	K	NIST Webbook

tb	345.05 ± 0.50	K	NIST Webbook
tb	344.65 ± 1.00	K	NIST Webbook
tb	344.48 ± 0.20	K	NIST Webbook
tb	344.53 ± 0.30	K	NIST Webbook
tb	344.00 ± 1.00	K	NIST Webbook
tb	344.15 ± 1.50	K	NIST Webbook
tb	344.15 ± 1.50	K	NIST Webbook
tb	343.45 ± 1.00	K	NIST Webbook
tb	344.80 ± 0.30	K	NIST Webbook
tb	344.70 ± 1.00	K	NIST Webbook
tb	344.80 ± 0.40	K	NIST Webbook
tb	344.70 ± 1.00	K	NIST Webbook
tb	344.49 ± 0.30	K	NIST Webbook
tb	344.50	K	NIST Webbook
tb	345.00 ± 1.00	K	NIST Webbook
tb	344.50	K	KDB
tb	343.35 ± 0.70	K	NIST Webbook
tb	344.52 ± 0.40	K	NIST Webbook
tb	344.70 ± 1.50	K	NIST Webbook
tc	529.00	K	KDB
tf	141.06 ± 0.10	K	NIST Webbook
tf	140.75 ± 0.40	K	NIST Webbook
tf	141.18	K	Aqueous Solubility Prediction Method
tf	141.00	K	KDB
tf	141.15 ± 1.50	K	NIST Webbook
vc	0.334	m3/kmol	KDB
zc	0.2797890		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.40	J/mol×K	414.34	Joback Method
cpg	156.26	J/mol×K	385.16	Joback Method
cpg	147.77	J/mol×K	355.98	Joback Method
cpg	186.81	J/mol×K	501.88	Joback Method
cpg	179.67	J/mol×K	472.70	Joback Method
cpg	172.20	J/mol×K	443.52	Joback Method
cpg	138.91	J/mol×K	326.80	Joback Method
hvapt	34.20	kJ/mol	262.00	NIST Webbook
hvapt	33.50	kJ/mol	270.00	NIST Webbook

hvapt	33.40	kJ/mol	328.00	NIST Webbook
pvap	2.72	kPa	263.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	96.32	kPa	343.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	68.90	kPa	333.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	48.09	kPa	323.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	32.65	kPa	313.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	21.50	kPa	303.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	17.22	kPa	298.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	13.67	kPa	293.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	8.36	kPa	283.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
pvap	4.89	kPa	273.15	Thermodynamics of isomeric hexynes +MTBE binary mixtures
rfi	1.39600		298.15	KDB

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	285.70	K	10.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46089e+01
Coeff. B	-3.07754e+03
Coeff. C	-3.64370e+01
Temperature range (K), min.	251.33
Temperature range (K), max.	367.45

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.50798e+01
Coeff. B	-6.95750e+03
Coeff. C	-1.22828e+01
Coeff. D	1.25260e-05
Temperature range (K), min.	141.25
Temperature range (K), max.	516.20

Sources

Thermodynamic Properties of Mixtures Containing Ionic Liquids: Activity Coefficients at Infinite Dilution of Organic Compounds in 1-Propyl Boronic Acid-3-Alkylimidazolium Bromide and 1-Propenyl-3-alkylimidazolium Bromide Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je060033f
Activity coefficients at infinite dilution of organic solutes in [illegible] based ionic liquids using gas-liquid chromatography:	https://www.doi.org/10.1016/j.jct.2015.02.023
Ammonium ionic liquids in extraction of bio-butan-1-ol from water phase using activity coefficients at infinite dilution	https://www.doi.org/10.1016/j.fluid.2018.09.024
Measurements of activity coefficients at infinite dilution of organic solutes and water in 1-propyl-1-methylpiperidinium bis{(trifluoromethyl)sulfonyl}imide ionic liquid using g.l.c.	https://www.doi.org/10.1016/j.jct.2010.05.017
Thermodynamics and activity coefficients at infinite dilution measurements for organic solutes and water in the ionic liquid 1-butyl-1-methylpyrrolidinium tetracyanoborate	https://www.doi.org/10.1016/j.jct.2011.06.007
Partition Coefficients of Organic Compounds in Four New Tetraalkylammonium Bis(trifluoromethylsulfonyl)imide Ionic Liquids Using Inverse Gas Chromatography	https://www.doi.org/10.1021/je200637v
NIST Webbook	http://webbook.nist.gov/cgi/cbook.cgi?ID=C693027&Units=SI
Measurements of Activity Coefficients at Infinite Dilution for Organic Solutes and Water in the Ionic Liquid 1-Butyl-1-methylpiperydinium Thiocyanate:	https://www.doi.org/10.1021/je101008y
Activity coefficients at infinite dilution of organic solutes in the ionic liquid 1-hexyl-3-methylimidazolium trifluoromethanesulfonate using gas liquid chromatography at T = (318.15, 328.15, and 338.15) K	https://www.doi.org/10.1016/j.jct.2009.07.010
Application of trihexyltetradecylphosphonium dicyanamide ionic liquid for various types of separation problems: Activity coefficients at infinite dilution measurements utilizing GLC method:	https://www.doi.org/10.1016/j.fluid.2019.03.023
Thermodynamics of isomeric hexynes + MTBE binary mixtures:	https://www.doi.org/10.1016/j.fluid.2006.08.007
Partition Coefficients of Organic Compounds in New Imidazolium and Tetraalkylammonium Based Ionic Liquids Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je9003178
Crippen Method	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Activity Coefficients at Infinite Dilution of Organic Compounds in 1-Butyl-3-methylimidazolium Tetrafluoroborate Using Inverse Gas Chromatography:	https://www.doi.org/10.1021/je800658v
Activity Coefficients at Infinite Dilution of Organic Solutes and Water in Tributylethylphosphonium Diethylphosphate Using Gas Liquid Chromatography: Thermodynamic Properties of Mixtures Containing Ionic Liquids:	https://www.doi.org/10.1021/acs.jced.5b00980

Separation of binary mixtures hexane/hex-1-ene, cyclohexane/cyclohexene and ethylbenzene/styrene based on gamma infinity data measurements	https://www.doi.org/10.1016/j.jct.2017.11.017
Activity coefficients at infinite dilution of organic solutes in the ionic liquid [illegible]	https://www.doi.org/10.1016/j.jct.2012.01.004
Activity coefficients at infinite dilution for organic solutes and water in [illegible] hexafluorophosphate using gas liquid chromatography [illegible]	https://www.doi.org/10.1016/j.jct.2015.05.014
Thermodynamic study of molecular interaction selectivity in separation processes based on limiting activity coefficients	https://www.doi.org/10.1016/j.jct.2018.02.014
Activity Coefficients at Infinite Dilution of Solutes in the Ionic Liquid 1-Hexyl-3-methylimidazolium Tetrafluoroborate Using Gas-Liquid Chromatography	https://www.doi.org/10.1021/je030187k
Determination of activity coefficients at infinite dilution of organic solutes in [illegible]	https://www.doi.org/10.1016/j.fluid.2006.03.002
Activity coefficients at infinite dilution and physicochemical properties for [illegible]	https://www.doi.org/10.1016/j.jct.2015.02.024
[illegible]	https://www.doi.org/10.1016/j.jct.2013.01.005
[illegible]	https://www.doi.org/10.1016/j.fluid.2017.06.001
[illegible]	https://www.doi.org/10.1016/j.jct.2012.09.033
[illegible] for organic solutes and water in a novel [illegible]	https://www.doi.org/10.1016/j.fluid.2010.08.016
Thermodynamics and limiting activity coefficients measurements for organic [illegible]	https://www.doi.org/10.1016/j.jct.2016.08.008
[illegible]	https://www.doi.org/10.1016/j.jct.2016.01.017
Activity coefficients at infinite dilution of organic solutes in the ionic liquid [illegible]	https://www.doi.org/10.1016/j.jct.2010.02.006
Activity coefficients at infinite dilution and physicochemical properties for [illegible]	https://www.doi.org/10.1016/j.jct.2011.11.021
Activity Coefficients at Infinite Dilution of Organic Compounds in [illegible]	https://www.doi.org/10.1021/je800754w
The study of activity coefficients at infinite dilution for organic solutes and [illegible]	https://www.doi.org/10.1016/j.jct.2013.09.007
[illegible]	https://www.doi.org/10.1016/j.jct.2014.12.027
Thermodynamics and activity coefficients at infinite dilution for [illegible]	https://www.doi.org/10.1016/j.jct.2014.04.024
Activity coefficients at infinite dilution of organic solutes in [illegible]	https://www.doi.org/10.1016/j.jct.2013.02.006
The use of ionic liquids for separation of binary hydrocarbons mixtures based on gamma infinity data measurements	https://www.doi.org/10.1016/j.jct.2018.07.024
[illegible] specific retention volumes and solvation thermodynamic [illegible]	https://www.doi.org/10.1016/j.fluid.2006.07.015
Activity coefficients at infinite dilution measurements for organic solutes and [illegible]	https://www.doi.org/10.1016/j.fluid.2009.01.011
Activity coefficients at infinite dilution and physicochemical properties for [illegible]	https://www.doi.org/10.1016/j.jct.2013.01.007
Activity coefficients at infinite dilution of organic solutes in N-alkylpyridinium [illegible]	https://www.doi.org/10.1016/j.jct.2010.06.009
Activity coefficients at infinite dilution [illegible]	https://www.doi.org/10.1016/j.jct.2004.03.001
[illegible] on activity coefficients at infinite dilution in [illegible]	https://www.doi.org/10.1016/j.jct.2017.10.003
Infinite Dilution Activity Coefficients of Solutes Dissolved in Two [illegible]	https://www.doi.org/10.1021/je500050p
Activity coefficients at infinite dilution measurements for organic solutes and water in the [illegible]	https://www.doi.org/10.1016/j.fluid.2009.08.017
Activity coefficients at infinite dilution measurements for organic solutes and [illegible]	https://www.doi.org/10.1016/j.jct.2009.06.011
Activity Coefficients at Infinite Dilution Measurements for Organic Solutes and [illegible]	https://www.doi.org/10.1021/je1000582
[illegible]	https://www.doi.org/10.1021/je900838a
Measurements of activity coefficients at infinite dilution of aliphatic and aromatic hydrocarbons, alcohols, [illegible]	https://www.doi.org/10.1016/j.jct.2008.12.018
Activity coefficients at infinite dilution measurements for organic solutes in [illegible]	https://www.doi.org/10.1016/j.jct.2005.01.015
[illegible]	https://www.doi.org/10.1016/j.jct.2015.05.022
[illegible]	https://www.doi.org/10.1016/j.fluid.2018.07.028
[illegible]	https://www.doi.org/10.1016/j.jct.2012.01.019
[illegible] and physicochemical properties for [illegible]	https://www.doi.org/10.1021/je201129y
Trigeminal Tricationic Ionic Liquids for [illegible]	https://www.doi.org/10.1021/je300692s
Activity Coefficients at Infinite Dilution for Organic Compounds Dissolved in [illegible]	https://www.doi.org/10.1016/j.jct.2013.08.030
[illegible]	https://www.doi.org/10.1016/j.jct.2010.12.020
[illegible]	https://www.doi.org/10.1016/j.fluid.2018.06.013
Infinite Dilution Activity Coefficients for Trihexyltetradecyl Phosphonium Ionic Liquids: Measurements and COSMO-RS Prediction:	https://www.doi.org/10.1021/je0602925

Determination of Activity Coefficients at Infinite Dilution of Solutes in the Ionic Liquid, …	https://www.doi.org/10.1021/je800105r
Activity Coefficients at Infinite Dilution Measurements for Organic Solutes and …	https://www.doi.org/10.1021/je900890u
Activity coefficients at infinite dilution of organic solutes in …	https://www.doi.org/10.1016/j.jct.2013.05.011
Separation of binary mixtures based on …	https://www.doi.org/10.1016/j.fluid.2017.12.029
Activity coefficients at infinite dilution measurements for organic solutes and …	https://www.doi.org/10.1016/j.jct.2011.02.012
Activity coefficients at infinite dilution measurements for organic solutes and …	https://www.doi.org/10.1016/j.jct.2008.12.005
Study of interaction between organic compounds and mono or dicationic …	https://www.doi.org/10.1016/j.fluid.2014.11.020
Measurements of activity coefficients at infinite dilution for organic solutes and water in the ionic liquid …	https://www.doi.org/10.1016/j.jct.2012.03.005
The determination of activity coefficients at infinite dilution using …	https://www.doi.org/10.1016/j.jct.2003.09.011
Activity coefficients at infinite dilution at T = …	https://www.doi.org/10.1016/j.jct.2009.12.004
Thermodynamics and selectivity of separation based on activity …	https://www.doi.org/10.1016/j.jct.2016.06.028
Activity coefficients at infinite dilution measurements for organic solutes in …	https://www.doi.org/10.1016/j.fluid.2008.10.008
Activity coefficients at infinite dilution and physicochemical properties for …	https://www.doi.org/10.1016/j.jct.2012.05.017
Relation between the characteristic …	https://www.doi.org/10.1016/j.jct.2010.04.011
Activity coefficients at infinite dilution of organic solutes in the ionic liquid …	https://www.doi.org/10.1016/j.jct.2010.12.005
…	http://link.springer.com/article/10.1007/BF02311772
Influence of High Pressure on the Liquidus Curve Shape in Binary Hydrocarbon Mixtures: Experimental Data, Correlation, and Prediction.	https://www.doi.org/10.1021/je050039p
Measurements of activity coefficients at infinite dilution …	https://www.doi.org/10.1016/j.jct.2010.01.004
Screening of environmental friendly ionic liquid as a solvent for the …	https://www.doi.org/10.1016/j.jct.2015.08.017
Activity Coefficients at Infinite Dilution … Hexafluorophosphate from Gas-Liquid Chromatography	https://www.doi.org/10.1021/je0256481
…	https://en.wikipedia.org/wiki/Joback_method
Measurement of activity coefficients at infinite dilution of organic solutes in …	https://www.doi.org/10.1016/j.jct.2013.10.017
Measurements of activity coefficients at infinite dilution of aromatic and …	https://www.doi.org/10.1016/j.jct.2008.01.004
Activity coefficients at infinite dilution of organic solutes in the ionic liquid …	https://www.doi.org/10.1016/j.jct.2010.12.019
Experimental and theoretical study of …	https://www.doi.org/10.1016/j.fluid.2014.06.021
Separation of binary mixtures …	https://www.doi.org/10.1016/j.jct.2017.03.004
Measurements of activity coefficients at infinite dilution for organic solutes …	https://www.doi.org/10.1016/j.jct.2013.02.004
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=407
Activity coefficients at infinite dilution for solutes in the …	https://www.doi.org/10.1016/j.jct.2009.08.012
Determination of Activity Coefficients at Infinite Dilution of Solutes in the …	https://www.doi.org/10.1021/je0500375
Measurement of activity coefficients at infinite dilution in …	https://www.doi.org/10.1016/j.jct.2007.01.004
Activity coefficients at infinite dilution …	https://www.doi.org/10.1016/j.fluid.2016.02.004
Activity Coefficients at Infinite Dilution …	https://www.doi.org/10.1021/je9008443
Determination of Activity Coefficients at Infinite Dilution of … Solutes in the …	https://www.doi.org/10.1021/je100410k
Determination of activity coefficients at infinite dilution of organic solutes in …	https://www.doi.org/10.1016/j.fluid.2005.04.021
KDB mol file:	https://www.cheric.org/files/research/kdb/mol/mol407.mol
Measurements of activity coefficients at infinite dilution of organic …	https://www.doi.org/10.1016/j.jct.2010.10.026
… coefficients at infinite dilution …	https://www.doi.org/10.1016/j.jct.2013.05.030
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Activity coefficients at infinite dilution measurements for organic solutes in …	https://www.doi.org/10.1016/j.jct.2005.03.014
Activity coefficients at infinite dilution and physicochemical properties for …	https://www.doi.org/10.1016/j.jct.2012.03.015
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Measurements of activity coefficients at infinite dilution for organic solutes in two quaternary ammonium-based ionic liquids [DDA][ClO4] and [DDA][BF4]:	https://www.doi.org/10.1016/j.fluid.2018.11.011

Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid trihexyl-tetradecyl-phosphonium tricyanomethanide:	https://www.doi.org/10.1016/j.jct.2018.01.003
Assessment of Pyrrolidinium-Based Ionic Liquid for the Separation of [illegible] Based on Activity Coefficients at Infinite Dilution:	https://www.doi.org/10.1021/acs.jced.9b00341
Measurements of activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-hexyl-3-methylimidazolium tetracyanoborate:	https://www.doi.org/10.1016/j.jct.2011.11.025
Determination of Activity Coefficients at Infinite Dilution of Organic Solutes in the Ionic Liquid 1-(2-Hydroxyethyl)-3-methylimidazolium Nonafluoro-1-butanesulfonate Using Gas-Liquid Chromatography:	https://www.doi.org/10.1021/acs.jced.8b00080
Activity coefficients at infinite dilution and physicochemical properties for [illegible]	https://www.doi.org/10.1016/j.jct.2011.04.018
Activity coefficients at infinite dilution [illegible]	https://www.doi.org/10.1016/j.jct.2013.05.008
Activity coefficients at infinite dilution measurements for organic solutes in [illegible]	https://www.doi.org/10.1016/j.jct.2008.04.002
Activity coefficients at infinite dilution and physicochemical properties for [illegible] bis(2,4,4-trimethylpentyl)-phosphinate [illegible]	https://www.doi.org/10.1016/j.jct.2012.08.016
Isothermal vapor-liquid equilibrium and excess enthalpies of binary mixtures of [illegible]	https://www.doi.org/10.1016/j.fluid.2010.10.022
Activity Coefficients at Infinite Dilution of Organic Compounds in Four New Imidazolium-Based Ionic Liquids:	https://www.doi.org/10.1021/je200195q
[illegible]	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Separation of aliphatic from aromatic hydrocarbons and sulphur compounds from fuel based on measurements of activity coefficients at infinite dilution [illegible]	https://www.doi.org/10.1016/j.jct.2016.07.017
Measurements of activity coefficients at infinite dilution for organic solutes and water in the [illegible] N,N-diethyl-N-methyl-N-(2-methoxyethyl)ammonium [illegible]	https://www.doi.org/10.1016/j.jct.2013.07.004
Determination of Activity Coefficients at Infinite Dilution of Polar and [illegible] 1-Ethyl-3-methylimidazolium Bis(trifluoromethylsulfonyl) Imidate Using Gas-Liquid Chromatography at the Temperature 303.15 K or 318.15 K:	https://www.doi.org/10.1021/je0498107
Activity Coefficients at Infinite Dilution of Organic Solutes Dissolved in Three 1-Alkyl-1-methylpyrrolidinium Bis(trifluoromethylsulfonyl)imide Ionic Liquids Bearing Short Linear Alkyl Side Chains of Three to Five Carbons:	https://www.doi.org/10.1021/je4001894

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hcg:	Heat of Combustion, Gross form
hcn:	Heat of Combustion, Net Form
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
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility