«alpha»-Methylstyrene

Other names:	(1-Methylethenyl)benzene
	(1-methylvinyl)benzene
	.alpha.-Methylstyrene
	1-Methyl-1-phenylethene
	1-Methyl-1-phenylethylene
	1-Phenyl-1-methylethylene
	1-Propene, 2-phenyl-
	2-Phenyl-1-propene
	2-Phenyl-2-propene
	2-Phenylpropene
	2-Phenylpropylene
	ALPHA-METHYLSTYRENE
	AS-Methylphenylethylene
	Benzene, (1-methylethenyl)-
	Benzene, isopropenyl-
	Isopropenil-benzolo
	Isopropenyl-benzeen
	Isopropenyl-benzol
	Isopropenylbenzene
	NSC 9400
	Styrene, «alpha»-methyl-
	Styrene, Â«alphaÂ»-methyl-
	UN 2303
	a-methylstyrene
	prop-1-en-2-ylbenzene
	styrene, .alpha.-methyl-
	«alpha»-Methylstyreen
	«alpha»-Methylstyrol
	«alpha»-Metil-stirolo
	«beta»-Phenylpropylene
	«beta»-phenylpropene
	Â«alphaÂ»-Methylstyreen
	Â«alphaÂ»-Methylstyrol
	Â«alphaÂ»-Metil-stirolo
	Â«betaÂ»-Phenylpropylene
	Â«betaÂ»-phenylpropene
Inchi:	InChI=1S/C9H10/c1-8(2)9-6-4-3-5-7-9/h3-7H,1H2,2H3
InchiKey:	XYLMUPLGERFSHI-UHFFFAOYSA-N
Formula:	C9H10
SMILES:	C=C(C)c1ccccc1

Mol. weight [g/mol]: 118.18
CAS: 98-83-9

Physical Properties

Property code	Value	Unit	Source
affp	864.20	kJ/mol	NIST Webbook
basg	835.30	kJ/mol	NIST Webbook
chg	-5083.77	kJ/mol	NIST Webbook
chl	-5093.20	kJ/mol	NIST Webbook
chl	-5000.30	kJ/mol	NIST Webbook
chl	-5041.18	kJ/mol	NIST Webbook
gf	216.60	kJ/mol	Joback Method
hf	118.30 ± 1.40	kJ/mol	NIST Webbook
hfus	10.52	kJ/mol	Joback Method
hvap	48.60 ± 0.40	kJ/mol	NIST Webbook
hvap	48.90 ± 0.30	kJ/mol	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.35 ± 0.01	eV	NIST Webbook
ie	8.18 ± 0.04	eV	NIST Webbook
ie	8.52	eV	NIST Webbook
ie	8.30 ± 0.10	eV	NIST Webbook
log10ws	-2.71		Crippen Method
logp	2.720		Crippen Method
mcvol	109.610	ml/mol	McGowan Method
pc	3550.00 ± 300.00	kPa	NIST Webbook
rhoc	288.35 ± 15.36	kg/m3	NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	964.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	974.00		NIST Webbook
rinpol	974.00		NIST Webbook

rinpol	964.90	NIST Webbook
rinpol	965.23	NIST Webbook
rinpol	987.90	NIST Webbook
rinpol	986.00	NIST Webbook
rinpol	963.50	NIST Webbook
rinpol	966.00	NIST Webbook
rinpol	967.00	NIST Webbook
rinpol	963.00	NIST Webbook
rinpol	968.00	NIST Webbook
rinpol	151.10	NIST Webbook
rinpol	980.00	NIST Webbook
rinpol	155.10	NIST Webbook
rinpol	155.89	NIST Webbook
rinpol	948.00	NIST Webbook
rinpol	980.00	NIST Webbook
rinpol	972.50	NIST Webbook
rinpol	963.10	NIST Webbook
rinpol	963.50	NIST Webbook
rinpol	963.10	NIST Webbook
rinpol	963.10	NIST Webbook
rinpol	963.20	NIST Webbook
rinpol	977.40	NIST Webbook
rinpol	963.10	NIST Webbook
rinpol	966.00	NIST Webbook
rinpol	948.00	NIST Webbook
rinpol	973.00	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	958.00	NIST Webbook
rinpol	966.40	NIST Webbook
rinpol	980.00	NIST Webbook
rinpol	968.00	NIST Webbook
rinpol	1016.00	NIST Webbook
rinpol	957.80	NIST Webbook
rinpol	960.00	NIST Webbook
rinpol	972.50	NIST Webbook
rinpol	963.10	NIST Webbook
rinpol	983.10	NIST Webbook
rinpol	957.80	NIST Webbook
rinpol	985.00	NIST Webbook
ripol	1363.00	NIST Webbook
ripol	1357.20	NIST Webbook
ripol	1366.00	NIST Webbook
ripol	1320.90	NIST Webbook
ripol	1353.30	NIST Webbook

ripol	1321.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1300.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1352.20		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1295.60		NIST Webbook
ripol	1294.70		NIST Webbook
ripol	1300.10		NIST Webbook
ripol	1351.40		NIST Webbook
sl	243.80	J/mol×K	NIST Webbook
tb	437.65 ± 1.50	K	NIST Webbook
tb	440.20	K	NIST Webbook
tb	438.60	K	NIST Webbook
tb	435.65 ± 10.00	K	NIST Webbook
tb	438.75 ± 0.50	K	NIST Webbook
tb	436.15 ± 3.00	K	NIST Webbook
tb	436.65 ± 2.00	K	NIST Webbook
tb	436.15 ± 3.00	K	NIST Webbook
tb	449.65	K	NIST Webbook
tb	438.68 ± 0.30	K	NIST Webbook
tb	438.53 ± 0.30	K	NIST Webbook
tb	434.15 ± 3.00	K	NIST Webbook
tb	438.70 ± 0.30	K	NIST Webbook
tb	438.15 ± 2.00	K	NIST Webbook
tb	438.65 ± 0.40	K	NIST Webbook
tb	443.15 ± 10.00	K	NIST Webbook
tc	645.00 ± 6.00	K	NIST Webbook
tf	249.94 ± 0.25	K	NIST Webbook
tf	247.22 ± 0.60	K	NIST Webbook
tf	249.05 ± 0.30	K	NIST Webbook
tf	244.83 ± 0.40	K	NIST Webbook
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.87	J/mol×K	608.77	Joback Method
cpg	198.91	J/mol×K	428.56	Joback Method
cpg	212.51	J/mol×K	464.60	Joback Method

cpg	225.28	J/mol×K	500.64	Joback Method
cpg	237.23	J/mol×K	536.69	Joback Method
cpg	248.41	J/mol×K	572.73	Joback Method
cpg	268.63	J/mol×K	644.81	Joback Method
cpl	202.20	J/mol×K	300.00	NIST Webbook
hfust	11.92	kJ/mol	250.80	NIST Webbook
hfust	11.92	kJ/mol	250.78	NIST Webbook
hvapt	44.80	kJ/mol	383.00	NIST Webbook
hvapt	49.20 ± 0.30	kJ/mol	294.00	NIST Webbook
hvapt	45.90 ± 0.30	kJ/mol	399.00	NIST Webbook
hvapt	43.30 ± 0.30	kJ/mol	399.00	NIST Webbook
hvapt	40.60 ± 0.30	kJ/mol	399.00	NIST Webbook
hvapt	37.70 ± 0.50	kJ/mol	399.00	NIST Webbook
hvapt	44.30	kJ/mol	418.00	NIST Webbook
sfust	47.55	J/mol×K	250.78	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.69992e+01
Coeff. B	-7.62172e+03
Coeff. C	-7.50767e+00
Coeff. D	3.35799e-06
Temperature range (K), min.	249.95
Temperature range (K), max.	654.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=719

Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

KDB:
4-(3-hydroxypropyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)-amide: https://www.cheric.org/files/research/kdb/mol/mol719.mol

Activity coefficients at infinite dilution and physicochemical properties for organic solutes and water in the ionic liquid
4-(2-methoxyethyl)-4-methylmorpholinium bis(trifluoromethylsulfonyl)-amide: https://www.doi.org/10.1016/j.jct.2011.11.021

Ammonium ionic liquids in extraction of bio-butan-1-ol from water phase
https://www.doi.org/10.1016/j.fluid.2018.09.024

Measurements of activity coefficients at infinite dilution for organic solutes and water in the ionic liquid 1-butyl-1-methylpyrrolidinium tricyanomethanide: https://www.doi.org/10.1016/j.jct.2013.07.004

Activity coefficients at infinite dilution measurements for 1-alkyl-1-methylpyrrolidinium-based ionic liquid in the separation processes: https://www.doi.org/10.1016/j.jct.2016.01.017

High selective water/butan-1-ol separation on investigation of limiting activity coefficients with	https://www.doi.org/10.1016/j.fluid.2017.06.001
Separation of binary mixtures based on limiting activity coefficients data using	https://www.doi.org/10.1016/j.fluid.2017.12.029
Separation of binary mixtures	https://www.doi.org/10.1016/j.jct.2017.03.004
hexane/hex-1-ene	
and modified of thermodynamic	
Activity coefficients at infinite dilution	https://www.doi.org/10.1016/j.jct.2012.01.019
and physicochemical properties for	
ethylbenzene/styrene based on limiting	https://www.doi.org/10.1016/j.jct.2012.03.005
activity coefficients.	
Measurements of activity coefficients	
at infinite dilution for organic solutes	
Physicochemical properties and	https://www.doi.org/10.1016/j.jct.2012.09.033
activity coefficients at infinite dilution	
1-(2-methoxyethyl)-1-methylpiperidinium	
bis(trifluoromethylsulfonyl)imide:	
Measurements of activity coefficients	https://www.doi.org/10.1016/j.jct.2013.08.030
at infinite dilution for organic solutes	
and water in a novel	
Activity coefficients at infinite dilution	https://www.doi.org/10.1016/j.jct.2013.05.008
and physicochemical properties for	
organic solutes and water in the ionic	
liquid 1-butyl-1-methylmorpholinium	
Activity coefficients at infinite dilution	https://www.doi.org/10.1016/j.jct.2012.05.017
and physicochemical properties for	
organic solutes and water in the ionic	
liquid 1-(2-methoxyethyl)-	
Crippen Method	https://www.chemeo.com/doc/models/crippen_log10ws
3-methylimidazolium	
tris(perfluoroethyl)trifluorophosphate:	
Activity coefficients at infinite dilution	https://www.doi.org/10.1016/j.jct.2012.08.016
and physicochemical properties for	
4-(2-methoxyethyl)-4-methylmorpholinium	
bis(trifluoromethylsulfonyl)imide:	
Activity coefficients at infinite dilution	http://link.springer.com/article/10.1007/BF02311772
and physicochemical properties for	
organic solutes and water in the ionic	
liquid 1-(2-methoxyethyl)-	
Activity coefficients at infinite dilution	https://www.doi.org/10.1016/j.jct.2012.03.015
and physicochemical properties for	
1-methylpiperidinium	
tris(pentafluoroethyl)trifluorophosphate:	
Thermodynamics and chromatographic	https://www.doi.org/10.1016/j.jct.2016.08.008
organic solutes and water in the ionic	
coefficients measurements for organic	
NIST Webbook	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98839&Units=SI
1-(2-methoxyethyl)-1-methylpyrrolidinium	
1-dodecyl-3-methylimidazolium	
bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.fluid.2018.07.028
bio-butanol extraction on investigation	
Thermodynamic study of molecular	https://www.doi.org/10.1016/j.jct.2018.02.014
interaction-selectivity in separation	
processes based on limiting activity	https://www.doi.org/10.1021/je050500d
coefficients.	
Measurements of activity coefficients	https://www.doi.org/10.1016/j.jct.2011.11.025
at infinite dilution for organic solutes	
Activity coefficients at infinite dilution,	https://www.doi.org/10.1016/j.jct.2015.05.022
physicochemical and thermodynamic	
1-hexyl-3-methylimidazolium	https://www.doi.org/10.1016/j.jct.2014.04.024
tetrafluoroborate and solvents and	
Activity coefficients at infinite dilution for	
organic solutes in the ionic liquid	https://www.doi.org/10.1016/j.jct.2018.07.024
The use of ionic liquids for separation	
Activity coefficients at infinite dilution	
bis(trifluoromethylsulfonyl)imide:	https://www.doi.org/10.1016/j.jct.2016.06.028
separation based on activity	
Activity coefficients at infinite dilution of	https://www.doi.org/10.1016/j.jct.2018.01.003
Activity coefficients at infinite dilution	
and physicochemical properties for	https://www.doi.org/10.1016/j.jct.2017.11.017
organic solutes and water in the ionic	
Liquid-liquid equilibrium of	https://www.doi.org/10.1016/j.fluid.2016.02.004
Activity coefficients at infinite dilution	
Activity coefficients at infinite dilution	https://www.doi.org/10.1016/j.jct.2013.01.007
and physicochemical properties for	
The study of activity coefficients at	https://www.doi.org/10.1016/j.jct.2013.09.007
infinite dilution for organic solutes and	
Joback Method	https://en.wikipedia.org/wiki/Joback_method
1-methylpyrrolidinium	
dicyanamide, [BMPyrr][DCA] using	
Separation of water/butan-1-ol based	https://www.doi.org/10.1016/j.jct.2017.10.003
GLC:	
Thermodynamics and activity	https://www.doi.org/10.1016/j.fluid.2018.06.013
coefficients at infinite dilution for	
organic solutes in the ionic liquid	
dicyanamide ionic liquid:	
1-butyl-1-methylpyrrolidinium	
dicyanamide:	

Legend

affp:	Proton affinity
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
gf:	Standard Gibbs free energy of formation

hf:	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
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume