Phenylethyne

Other names:	1-Phenylethyne
	Acetylene, phenyl-
	Benzene, ethynyl-
	Ethinylbenzene
	Ethyne, phenyl-
	Ethynylbenzene
	Phenylacetylene
Inchi:	InChI=1S/C8H6/c1-2-8-6-4-3-5-7-8/h1,3-7H
InchiKey:	UEXCJVNBTNXOEH-UHFFFAOYSA-N
Formula:	C8H6
SMILES:	C#Cc1ccccc1
Mol. weight [g/mol]:	102.13
CAS:	536-74-3

Physical Properties

Property code	Value	Unit	Source
affp	828.90	kJ/mol	NIST Webbook
affp	832.00	kJ/mol	NIST Webbook
basg	801.30	kJ/mol	NIST Webbook
basg	798.70	kJ/mol	NIST Webbook
chl	-4289.90	kJ/mol	NIST Webbook
gf	351.96	kJ/mol	Joback Method
hf	306.60 ± 1.70	kJ/mol	NIST Webbook
hfl	-261.00	kJ/mol	NIST Webbook
hfl	284.30 ± 4.00	kJ/mol	NIST Webbook
hfus	13.49	kJ/mol	Joback Method
hvap	35.54	kJ/mol	Joback Method
ie	8.82 ± 0.02	eV	NIST Webbook
ie	8.82 ± 0.00	eV	NIST Webbook
ie	8.81 ± 0.01	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	8.75	eV	NIST Webbook
ie	8.88 ± 0.02	eV	NIST Webbook
ie	9.56 ± 0.02	eV	NIST Webbook
ie	8.78	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.82 ± 0.02	eV	NIST Webbook

ie	8.78	eV	NIST Webbook
ie	8.82 ± 0.08	eV	NIST Webbook
log10ws	-2.17		Crippen Method
logp	1.668		Crippen Method
mcvol	91.220	ml/mol	McGowan Method
pc	4403.25	kPa	Joback Method
rinpol	870.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	830.40		NIST Webbook
rinpol	834.10		NIST Webbook
rinpol	830.40		NIST Webbook
rinpol	834.10		NIST Webbook
rinpol	830.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	877.00		NIST Webbook
rinpol	875.90		NIST Webbook
rinpol	856.00		NIST Webbook
rinpol	849.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	122.00		NIST Webbook
rinpol	122.10		NIST Webbook
rinpol	122.70		NIST Webbook
rinpol	881.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	833.00		NIST Webbook
rinpol	862.10		NIST Webbook
ripol	1354.00		NIST Webbook
ripol	1357.20		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1357.20		NIST Webbook
ripol	1370.00		NIST Webbook
ripol	1372.00		NIST Webbook
sl	221.20	J/mol×K	NIST Webbook
tb	415.65 ± 1.50	K	NIST Webbook
tb	412.65 ± 1.50	K	NIST Webbook
tb	414.65 ± 3.00	K	NIST Webbook
tb	416.20	K	NIST Webbook
tb	416.00 ± 1.00	K	NIST Webbook
tc	625.47	K	Joback Method

tf	228.35 ± 0.40	K	NIST Webbook
tt	228.04 ± 0.02	K	NIST Webbook
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.33	J/mol×K	587.77	Joback Method
cpg	160.67	J/mol×K	436.95	Joback Method
cpg	170.89	J/mol×K	474.65	Joback Method
cpg	180.38	J/mol×K	512.36	Joback Method
cpg	189.18	J/mol×K	550.06	Joback Method
cpg	204.88	J/mol×K	625.47	Joback Method
cpg	149.68	J/mol×K	399.24	Joback Method
cpl	179.50	J/mol×K	298.50	NIST Webbook
cpl	180.10	J/mol×K	298.15	NIST Webbook
hfust	9.46	kJ/mol	228.00	NIST Webbook
hfust	9.46	kJ/mol	228.04	NIST Webbook
hfust	9.46	kJ/mol	228.00	NIST Webbook
hvapt	45.20	kJ/mol	281.00	NIST Webbook
hvapt	43.90	kJ/mol	278.00	NIST Webbook
hvapt	38.00 ± 0.20	kJ/mol	364.50	NIST Webbook
hvapt	40.40 ± 0.10	kJ/mol	364.50	NIST Webbook
hvapt	42.60 ± 0.10	kJ/mol	364.50	NIST Webbook
sfust	41.50	J/mol×K	228.04	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72233e+01
Coeff. B	-4.13406e+03
Coeff. C	-7.16380e+01
Temperature range (K), min.	315.74
Temperature range (K), max.	418.69

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C536743&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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
pc:	Critical Pressure
pvap:	Vapor pressure
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
tt:	Triple Point Temperature
vc:	Critical Volume