Benzene-D6

Other names:	(2H6)benzene
	D6-Benzene
	hexadeuteriobenzene
	hexadeuterobenzene
	perdeuteriobenzene
	perdeuterobenzene
Inchi:	InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H/i1D,2D,3D,4D,5D,6D
InchiKey:	UHOVQNZJYSORNB-MZWXYZOWSA-N
Formula:	C6D6
SMILES:	c1ccccc1
Mol. weight [g/mol]:	84.15
CAS:	1076-43-3

Physical Properties

Property code	Value	Unit	Source
gf	121.68	kJ/mol	Joback Method
hf	80.83	kJ/mol	Joback Method
hfus	5.73	kJ/mol	Joback Method
hvap	34.20	kJ/mol	NIST Webbook
ie	9.25 ± 0.01	eV	NIST Webbook
ie	9.25 ± 0.00	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
ie	9.25 ± 0.01	eV	NIST Webbook
log10ws	-1.47		Crippen Method
logp	1.687		Crippen Method
mcvol	71.640	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
tb	345.43 ± 0.10	K	NIST Webbook
tc	569.71	K	Joback Method
tf	280.00 ± 0.30	K	NIST Webbook
tt	279.90 ± 0.10	K	NIST Webbook
vc	0.264	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	101.52	J/mol×K	358.38	Joback Method
cpg	121.98	J/mol×K	428.82	Joback Method
cpg	131.23	J/mol×K	464.04	Joback Method
cpg	139.87	J/mol×K	499.27	Joback Method
cpg	147.93	J/mol×K	534.49	Joback Method
cpg	155.43	J/mol×K	569.71	Joback Method
cpg	112.09	J/mol×K	393.60	Joback Method
cpl	149.40	J/mol×K	298.50	NIST Webbook
cpl	152.46	J/mol×K	298.00	NIST Webbook
dvisc	0.0018111	Pa×s	202.46	Joback Method
dvisc	0.0009618	Pa×s	233.65	Joback Method
dvisc	0.0005929	Pa×s	264.83	Joback Method
dvisc	0.0004047	Pa×s	296.01	Joback Method
dvisc	0.0002971	Pa×s	327.20	Joback Method
dvisc	0.0002301	Pa×s	358.38	Joback Method
dvisc	0.0042941	Pa×s	171.28	Joback Method
hfust	9.79	kJ/mol	279.85	NIST Webbook
hfust	9.79	kJ/mol	279.90	NIST Webbook
hvapt	33.25	kJ/mol	298.00	Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Hydrocarbons. Liquid-Vapor Pressure Isotope Effects
sfust	34.99	J/mol×K	279.85	NIST Webbook
tcondl	0.13	W/m×K	304.05	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.13	W/m×K	316.89	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	316.66	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	316.34	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	304.59	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	304.37	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

tcondl	0.13	W/m×K	326.75	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	292.04	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	291.83	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	291.53	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/m×K	281.26	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

tcondl	0.14	W/m×K	281.06	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.14	W/m×K	280.76	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.13	W/m×K	327.08	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	
tcondl	0.12	W/m×K	327.31	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons	

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons:	https://www.doi.org/10.1021/je034162x
Enthalpies of Vaporization and Vapor Pressures of Some Deuterated Isotope Effects:	https://www.doi.org/10.1021/je800091s
Joback Method	https://en.wikipedia.org/wiki/Joback_method
Liquid-Vapor Pressure	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1076433&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tcondl:	Liquid thermal conductivity
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume