

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 ± 0.01	eV	NIST Webbook
ie	9.25	eV	NIST Webbook
ie	9.25 ± 0.00	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	Paxs	202.46	Joback Method
dvisc	0.0009618	Paxs	233.65	Joback Method
dvisc	0.0005929	Paxs	264.83	Joback Method
dvisc	0.0004047	Paxs	296.01	Joback Method
dvisc	0.0002971	Paxs	327.20	Joback Method
dvisc	0.0002301	Paxs	358.38	Joback Method
dvisc	0.0042941	Paxs	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/mxK	316.89	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/mxK	316.66	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/mxK	316.34	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/mxK	304.59	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/mxK	304.37	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons

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

tcondl	0.14	W/mxK	281.06	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.14	W/mxK	280.76	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.13	W/mxK	327.08	Thermal Conductivity and Thermal Diffusivity of Twenty-Nine Liquids: Alkenes, Cyclic (Alkanes, Alkenes, Alkadienes, Aromatics), and Deuterated Hydrocarbons
tcondl	0.12	W/mxK	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: Liquid-Vapor Pressure Isotope Effects: McGowan Method

<https://www.doi.org/10.1021/je034162x>

<https://www.doi.org/10.1021/je800091s>

https://en.wikipedia.org/wiki/Joback_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

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