Diphenylmethane

Other names:	1,1'-Dimethylenebis(benzene) ALPHA-PHENYLTOLUENE BENZYLBENZENE Benzene, (phenylmethyl)- Benzene, 1,1'-methylenebis- Benzene, benzyl- DITAN Ditane Methane, diphenyl- NSC 4708 Toluene, «alpha»-phenyl- Toluene, Â«alphaÂ»-phenyl- phenylmethylbenzene
Inchi:	InChI=1S/C13H12/c1-3-7-12(8-4-1)11-13-9-5-2-6-10-13/h1-10H,11H2
InchiKey:	CZZYITDELCSZES-UHFFFAOYSA-N
Formula:	C13H12
SMILES:	c1ccc(Cc2ccccc2)cc1
Mol. weight [g/mol]:	168.23
CAS:	101-81-5

Physical Properties

Property code	Value	Unit	Source
af	0.4420		KDB
affp	802.00	kJ/mol	NIST Webbook
basg	769.50	kJ/mol	NIST Webbook
chl	-6927.20 ± 1.40	kJ/mol	NIST Webbook
chl	-6919.60 ± 1.30	kJ/mol	NIST Webbook
chs	-6929.54 ± 0.84	kJ/mol	NIST Webbook
chs	-6945.00	kJ/mol	NIST Webbook
chs	-6673.00	kJ/mol	NIST Webbook
chs	-6931.20	kJ/mol	NIST Webbook
dm	0.40	debye	KDB
ea	0.16 ± 0.04	eV	NIST Webbook
gf	283.40	kJ/mol	Joback Method
hf	165.00 ± 2.20	kJ/mol	NIST Webbook
hf	164.80 ± 1.60	kJ/mol	NIST Webbook
hf	162.30 ± 2.30	kJ/mol	NIST Webbook

hf	156.60	kJ/mol	NIST Webbook
hfl	97.10 ± 2.20	kJ/mol	NIST Webbook
hfl	88.91	kJ/mol	NIST Webbook
hfl	97.10 ± 1.40	kJ/mol	NIST Webbook
hfs	75.10 ± 2.20	kJ/mol	NIST Webbook
hfs	114.00	kJ/mol	NIST Webbook
hfus	19.01	kJ/mol	Thermodynamic Properties of Diphenylmethane
hsub	87.60 ± 0.80	kJ/mol	NIST Webbook
hsub	87.20 ± 0.70	kJ/mol	NIST Webbook
hvap	67.70	kJ/mol	NIST Webbook
hvap	67.60 ± 0.20	kJ/mol	NIST Webbook
hvap	67.90 ± 0.40	kJ/mol	NIST Webbook
hvap	66.60 ± 0.10	kJ/mol	NIST Webbook
hvap	64.70 ± 0.20	kJ/mol	NIST Webbook
hvap	67.90 ± 0.50	kJ/mol	NIST Webbook
hvap	65.70	kJ/mol	NIST Webbook
hvap	50.12	kJ/mol	NIST Webbook
hvap	67.70 ± 0.60	kJ/mol	NIST Webbook
hvap	67.50 ± 0.30	kJ/mol	NIST Webbook
ie	9.10	eV	NIST Webbook
ie	8.55 ± 0.03	eV	NIST Webbook
ie	8.80 ± 0.02	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.67 ± 0.05	eV	NIST Webbook
ie	9.00 ± 0.05	eV	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
ie	9.40	eV	NIST Webbook
log10ws	-4.08		Estimated Solubility Method
log10ws	-4.12		Aqueous Solubility Prediction Method
logp	3.277		Crippen Method
mcvol	146.510	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
nfpah	%!d(float64=1)		KDB
pc	2710.00 ± 300.00	kPa	NIST Webbook
pc	2857.36 ± 101.32	kPa	NIST Webbook
pc	5978.17 ± 303.98	kPa	NIST Webbook
pc	2700.00 ± 300.00	kPa	NIST Webbook
pc	2710.00	kPa	KDB
pc	2857.36 ± 101.32	kPa	NIST Webbook
rhoc	299.46 ± 20.19	kg/m3	NIST Webbook
rhoc	302.82 ± 50.47	kg/m3	NIST Webbook

rinpol	249.09	NIST Webbook
rinpol	243.40	NIST Webbook
rinpol	247.00	NIST Webbook
rinpol	1405.20	NIST Webbook
rinpol	1424.00	NIST Webbook
rinpol	1429.40	NIST Webbook
rinpol	1448.70	NIST Webbook
rinpol	245.60	NIST Webbook
rinpol	1400.00	NIST Webbook
rinpol	245.60	NIST Webbook
rinpol	1412.00	NIST Webbook
rinpol	243.35	NIST Webbook
rinpol	245.56	NIST Webbook
rinpol	245.60	NIST Webbook
rinpol	243.40	NIST Webbook
rinpol	245.77	NIST Webbook
rinpol	249.09	NIST Webbook
rinpol	241.60	NIST Webbook
rinpol	247.00	NIST Webbook
rinpol	1461.00	NIST Webbook
rinpol	1403.00	NIST Webbook
rinpol	1416.00	NIST Webbook
rinpol	1380.10	NIST Webbook
rinpol	1393.00	NIST Webbook
rinpol	1400.00	NIST Webbook
rinpol	1406.00	NIST Webbook
rinpol	1401.00	NIST Webbook
rinpol	1412.00	NIST Webbook
rinpol	1389.60	NIST Webbook
rinpol	1380.10	NIST Webbook
rinpol	1403.90	NIST Webbook
rinpol	1418.10	NIST Webbook
rinpol	1405.20	NIST Webbook
rinpol	1458.00	NIST Webbook
rinpol	1449.00	NIST Webbook
rinpol	1415.00	NIST Webbook
rinpol	1429.40	NIST Webbook
rinpol	1412.40	NIST Webbook
rinpol	1429.80	NIST Webbook
rinpol	1423.50	NIST Webbook
rinpol	1414.60	NIST Webbook
rinpol	1424.00	NIST Webbook
rinpol	1448.70	NIST Webbook
ripol	1994.00	NIST Webbook

ripol	1980.00		NIST Webbook
ripol	1994.00		NIST Webbook
ripol	1994.00		NIST Webbook
ripol	1984.00		NIST Webbook
ripol	1980.00		NIST Webbook
sg	436.00	J/mol×K	NIST Webbook
ss	239.30	J/mol×K	NIST Webbook
tb	533.00 ± 5.00	K	NIST Webbook
tb	534.00 ± 4.00	K	NIST Webbook
tb	536.00 ± 4.00	K	NIST Webbook
tb	534.00 ± 3.00	K	NIST Webbook
tb	536.00 ± 6.00	K	NIST Webbook
tb	537.85 ± 1.00	K	NIST Webbook
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tb	534.00 ± 3.00	K	NIST Webbook
tb	538.20	K	KDB
tb	538.00 ± 3.00	K	NIST Webbook
tb	537.50	K	NIST Webbook
tb	534.70 ± 2.00	K	NIST Webbook
tb	534.00 ± 3.00	K	NIST Webbook
tb	537.42 ± 0.20	K	NIST Webbook
tb	536.00 ± 0.50	K	NIST Webbook
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tb	535.65 ± 4.00	K	NIST Webbook
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tb	533.00 ± 4.00	K	NIST Webbook
tb	534.00 ± 3.00	K	NIST Webbook

tb	537.00 ± 3.00	K	NIST Webbook
tb	538.80 ± 1.50	K	NIST Webbook
tb	529.00 ± 5.00	K	NIST Webbook
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tb	537.00	K	NIST Webbook
tc	770.20 ± 10.00	K	NIST Webbook
tc	770.15 ± 2.00	K	NIST Webbook
tc	845.65 ± 3.00	K	NIST Webbook
tc	760.00 ± 8.00	K	NIST Webbook
tc	767.00 ± 10.00	K	NIST Webbook
tc	760.00 ± 8.00	K	NIST Webbook
tc	760.00	K	KDB
tc	760.00 ± 8.00	K	NIST Webbook
tf	298.00 ± 3.00	K	NIST Webbook
tf	571.40 ± 0.30	K	NIST Webbook
tf	298.21 ± 0.15	K	NIST Webbook
tf	298.17 ± 0.10	K	NIST Webbook
tf	300.20 ± 0.70	K	NIST Webbook
tf	298.20 ± 1.00	K	NIST Webbook
tf	298.35 ± 0.15	K	NIST Webbook
tf	298.80 ± 3.00	K	NIST Webbook
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tf	299.65 ± 0.50	K	NIST Webbook
tf	298.30 ± 0.30	K	NIST Webbook
tf	25.20 ± 0.20	K	NIST Webbook
tf	299.00 ± 2.00	K	NIST Webbook
tf	299.80 ± 0.50	K	NIST Webbook
tf	298.25 ± 0.30	K	NIST Webbook
tf	314.32	K	Aqueous Solubility Prediction Method
tf	300.15 ± 2.00	K	NIST Webbook
tf	298.40 ± 3.00	K	NIST Webbook
tf	301.00 ± 3.00	K	NIST Webbook
tf	298.00 ± 0.70	K	NIST Webbook
tf	299.00 ± 2.00	K	NIST Webbook

tf	298.24 ± 0.02	K	NIST Webbook
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tf	299.00 ± 3.00	K	NIST Webbook
tf	298.39	K	KDB
tf	300.00 ± 2.00	K	NIST Webbook
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tf	299.70 ± 1.50	K	NIST Webbook
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tf	298.80 ± 1.50	K	NIST Webbook
tf	299.50 ± 1.50	K	NIST Webbook
tf	299.80 ± 1.50	K	NIST Webbook
tf	298.00 ± 3.00	K	NIST Webbook
tf	299.00 ± 3.00	K	NIST Webbook
tf	299.00 ± 3.00	K	NIST Webbook
tf	299.00 ± 3.00	K	NIST Webbook
tf	297.70 ± 3.00	K	NIST Webbook
tf	299.70 ± 3.00	K	NIST Webbook
tf	298.00 ± 2.00	K	NIST Webbook
tf	299.60 ± 2.00	K	NIST Webbook
tf	299.00 ± 3.00	K	NIST Webbook
vc	0.563	m3/kmol	NIST Webbook
vc	0.563	m3/kmol	KDB
zc	0.2414500		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.47	J/mol×K	713.31	Joback Method
cpg	397.73	J/mol×K	754.08	Joback Method
cpg	324.65	J/mol×K	550.20	Joback Method
cpg	341.78	J/mol×K	590.98	Joback Method
cpg	357.57	J/mol×K	631.75	Joback Method
cpg	372.11	J/mol×K	672.53	Joback Method
cpg	408.98	J/mol×K	794.86	Joback Method
cps	279.90	J/mol×K	300.00	NIST Webbook
cps	233.50	J/mol×K	298.50	NIST Webbook
cps	223.80	J/mol×K	282.50	NIST Webbook
cps	266.10	J/mol×K	303.00	NIST Webbook
dvisc	0.0026514	Pa×s	289.11	Joback Method

dvisc	0.0007360	Pa×s	376.14	Joback Method
dvisc	0.0004733	Pa×s	419.66	Joback Method
dvisc	0.0003307	Pa×s	463.17	Joback Method
dvisc	0.0002458	Pa×s	506.69	Joback Method
dvisc	0.0001914	Pa×s	550.20	Joback Method
dvisc	0.0012846	Pa×s	332.62	Joback Method
hfust	18.58	kJ/mol	298.30	NIST Webbook
hfust	18.57	kJ/mol	298.30	NIST Webbook
hfust	19.01	kJ/mol	298.40	NIST Webbook
hfust	19.05	kJ/mol	299.40	NIST Webbook
hfust	18.58	kJ/mol	298.30	NIST Webbook
hsubt	88.50 ± 0.80	kJ/mol	284.00	NIST Webbook
hsubt	71.50	kJ/mol	285.50	NIST Webbook
hsubt	83.30 ± 3.30	kJ/mol	285.50	NIST Webbook
hsubt	82.47 ± 0.63	kJ/mol	299.80	NIST Webbook
hsubt	64.00	kJ/mol	288.50	NIST Webbook
hsubt	72.00 ± 0.80	kJ/mol	297.00	NIST Webbook
hsubt	72.00 ± 0.80	kJ/mol	297.00	NIST Webbook
hvapt	61.00 ± 0.10	kJ/mol	459.00	NIST Webbook
hvapt	57.90 ± 0.10	kJ/mol	459.00	NIST Webbook
hvapt	64.10 ± 0.10	kJ/mol	459.00	NIST Webbook
hvapt	55.00 ± 0.10	kJ/mol	459.00	NIST Webbook
hvapt	52.00 ± 0.20	kJ/mol	459.00	NIST Webbook
hvapt	48.90 ± 0.30	kJ/mol	459.00	NIST Webbook
hvapt	66.40 ± 0.50	kJ/mol	323.00	NIST Webbook
hvapt	61.80	kJ/mol	393.00	NIST Webbook
hvapt	63.70	kJ/mol	352.50	NIST Webbook
hvapt	72.20	kJ/mol	339.00	NIST Webbook
hvapt	55.80	kJ/mol	445.00	NIST Webbook
hvapt	49.00	kJ/mol	535.00	NIST Webbook
hvapt	54.20	kJ/mol	522.50	NIST Webbook
hvapt	56.70	kJ/mol	503.00	NIST Webbook
pvap	3.11	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	22.63	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	29.69	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	
pvap	38.42	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	
pvap	49.08	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	
pvap	17.00	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	
pvap	12.56	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	
pvap	9.12	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	
pvap	6.50	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons	

pvap	4.55	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.08	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.35	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.86	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.53	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.31	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.18	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.10	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.05	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.03	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.01	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.64e-03	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.39e-03	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.02e-03	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	510.00	kPa	623.10	A novel continuous flow apparatus with a video camera system for high pressure phase equilibrium measurements
pvap	520.00	kPa	623.10	A novel continuous flow apparatus with a video camera system for high pressure phase equilibrium measurements
pvap	510.00	kPa	623.00	A novel continuous flow apparatus with a video camera system for high pressure phase equilibrium measurements
pvap	340.00	kPa	598.00	A novel continuous flow apparatus with a video camera system for high pressure phase equilibrium measurements
pvap	330.00	kPa	598.00	A novel continuous flow apparatus with a video camera system for high pressure phase equilibrium measurements
pvap	330.00	kPa	598.00	A novel continuous flow apparatus with a video camera system for high pressure phase equilibrium measurements
pvap	210.00	kPa	573.10	A novel continuous flow apparatus with a video camera system for high pressure phase equilibrium measurements

pvap	210.00	kPa	573.10	A novel continuous flow apparatus with a video camera system for high pressure phase equilibrium measurements
pvap	200.00	kPa	573.10	A novel continuous flow apparatus with a video camera system for high pressure phase equilibrium measurements
rhol	1006.00	kg/m3	293.00	KDB
sfust	62.34	J/mol×K	298.30	NIST Webbook
sfust	62.25	J/mol×K	298.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48830e+01
Coeff. B	-4.71056e+03
Coeff. C	-7.60920e+01
Temperature range (K), min.	398.83
Temperature range (K), max.	568.23

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.11780e+02
Coeff. B	-1.19847e+04
Coeff. C	-1.37414e+01
Coeff. D	5.26072e-06
Temperature range (K), min.	298.39
Temperature range (K), max.	768.00

Sources

A novel continuous flow apparatus with a video camera system for high pressure phase equilibrium measurements:	https://www.doi.org/10.1016/j.fluid.2013.07.001
Thermodynamic Properties of Diphenylmethane:	https://www.doi.org/10.1021/je050034s
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=781
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
KDB:	https://www.cheric.org/files/research/kdb/mol/mol781.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101815&Units=SI
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
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
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation 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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility