Bibenzyl

Other names:	1,2-Diphenylethane 1,2-Diphenylethane(sym) 1,2-Diphenylethane, s 2-phenylethylbenzene Benzene, (phenylethyl)- Benzene, 1,1'-(1,2-ethanediyl)bis- DIBENZIL DIHYDROSTILBENE Dibenzyl Ethane, 1,2-diphenyl- NSC 30686 s-Diphenylethane sym-Diphenylethane
Inchi:	InChI=1S/C14H14/c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-14/h1-10H,11-12H2
InchiKey:	QWUWMCYKGHVNAV-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	c1ccc(CCc2ccccc2)cc1
Mol. weight [g/mol]:	182.26
CAS:	103-29-7

Physical Properties

Property code	Value	Unit	Source
affp	801.80	kJ/mol	NIST Webbook
basg	774.10	kJ/mol	NIST Webbook
chl	-7562.60 ± 7.50	kJ/mol	NIST Webbook
chs	-7559.60 ± 1.00	kJ/mol	NIST Webbook
chs	-7561.50 ± 1.10	kJ/mol	NIST Webbook
chs	-7554.80 ± 3.00	kJ/mol	NIST Webbook
chs	-7594.40	kJ/mol	NIST Webbook
chs	-7280.00	kJ/mol	NIST Webbook
gf	291.82	kJ/mol	Joback Method
hf	129.00	kJ/mol	NIST Webbook
hf	135.60 ± 1.30	kJ/mol	NIST Webbook
hfs	51.50 ± 1.30	kJ/mol	NIST Webbook
hfs	44.90 ± 3.10	kJ/mol	NIST Webbook
hfus	20.10	kJ/mol	Joback Method
hsub	91.38 ± 0.46	kJ/mol	NIST Webbook

hsub	91.50 ± 0.70	kJ/mol	NIST Webbook
hsub	91.40 ± 0.50	kJ/mol	NIST Webbook
hsub	84.10	kJ/mol	NIST Webbook
hsub	73.20 ± 0.80	kJ/mol	NIST Webbook
hvap	51.31	kJ/mol	Joback Method
ie	9.10	eV	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
ie	9.00 ± 0.05	eV	NIST Webbook
log10ws	-4.62		Aqueous Solubility Prediction Method
log10ws	-4.62		Estimated Solubility Method
logp	3.472		Crippen Method
mcvol	160.600	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	260.49		NIST Webbook
rinpol	1524.30		NIST Webbook
rinpol	1509.30		NIST Webbook
rinpol	260.10		NIST Webbook
rinpol	1496.70		NIST Webbook
rinpol	260.10		NIST Webbook
rinpol	1546.30		NIST Webbook
rinpol	258.90		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1508.80		NIST Webbook
rinpol	1519.20		NIST Webbook
rinpol	1524.30		NIST Webbook
rinpol	1508.80		NIST Webbook
rinpol	1519.20		NIST Webbook
rinpol	1524.30		NIST Webbook
rinpol	1528.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1487.00		NIST Webbook
rinpol	260.40		NIST Webbook
rinpol	260.13		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1508.80		NIST Webbook
ripol	2070.00		NIST Webbook
ripol	2061.00		NIST Webbook
ripol	2061.00		NIST Webbook
ripol	2072.00		NIST Webbook

ripol	2069.00		NIST Webbook
ss	270.30	J/mol×K	NIST Webbook
ss	267.39	J/mol×K	NIST Webbook
tb	573.08	K	Joback Method
tc	812.67	K	Joback Method
tf	325.77	K	Aqueous Solubility Prediction Method
tf	324.95	K	KDB
tt	324.34 ± 0.01	K	NIST Webbook
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.35	J/mol×K	812.67	Joback Method
cpg	390.10	J/mol×K	613.01	Joback Method
cpg	406.52	J/mol×K	652.94	Joback Method
cpg	421.67	J/mol×K	692.87	Joback Method
cpg	435.64	J/mol×K	732.81	Joback Method
cpg	448.51	J/mol×K	772.74	Joback Method
cpg	372.34	J/mol×K	573.08	Joback Method
cps	320.10	J/mol×K	330.00	NIST Webbook
cps	251.90	J/mol×K	298.10	NIST Webbook
cps	257.00	J/mol×K	303.00	NIST Webbook
cps	253.60	J/mol×K	298.50	NIST Webbook
cps	251.00	J/mol×K	293.60	NIST Webbook
cps	253.76	J/mol×K	298.15	NIST Webbook
dvisc	0.0001783	Pa×s	573.08	Joback Method
dvisc	0.0002301	Pa×s	527.63	Joback Method
dvisc	0.0003115	Pa×s	482.18	Joback Method
dvisc	0.0004491	Pa×s	436.73	Joback Method
dvisc	0.0007050	Pa×s	391.28	Joback Method
dvisc	0.0026164	Pa×s	300.38	Joback Method
dvisc	0.0012460	Pa×s	345.83	Joback Method
hfust	22.73	kJ/mol	324.30	NIST Webbook
hfust	2.25	kJ/mol	273.20	NIST Webbook
hfust	22.57	kJ/mol	324.30	NIST Webbook
hfust	23.01	kJ/mol	324.40	NIST Webbook
hfust	22.73	kJ/mol	324.30	NIST Webbook
hsubt	72.40 ± 1.30	kJ/mol	303.50	NIST Webbook
hsubt	84.10 ± 0.40	kJ/mol	296.50	NIST Webbook

hsubt	83.97 ± 0.46	kJ/mol	326.20	NIST Webbook
hsubt	92.90	kJ/mol	308.00	NIST Webbook
hsubt	91.20 ± 0.40	kJ/mol	295.50	NIST Webbook
hvapt	66.20 ± 0.20	kJ/mol	340.00	NIST Webbook
hvapt	57.00	kJ/mol	458.00	NIST Webbook
hvapt	67.40	kJ/mol	398.00	NIST Webbook
hvapt	64.10	kJ/mol	373.00	NIST Webbook
hvapt	67.53 ± 0.10	kJ/mol	324.40	NIST Webbook
sfust	70.90	J/mol×K	324.40	NIST Webbook
sfust	70.09	J/mol×K	324.30	NIST Webbook
sfust	8.23	J/mol×K	273.20	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46161e+01
Coeff. B	-4.80619e+03
Coeff. C	-7.52760e+01
Temperature range (K), min.	410.70
Temperature range (K), max.	591.81

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.13283e+02
Coeff. B	-1.22009e+04
Coeff. C	-1.39952e+01
Coeff. D	5.69580e-06
Temperature range (K), min.	324.34
Temperature range (K), max.	780.00

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=793

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol793.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103297&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid 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