

Benzene, 1,1'-hexylidenebis-

Other names:	1,1-Diphenylhexane
Inchi:	InChI=1S/C18H22/c1-2-3-6-15-18(16-11-7-4-8-12-16)17-13-9-5-10-14-17/h4-5,7-14,18H
InchiKey:	BXINIXQKBCSKKR-UHFFFAOYSA-N
Formula:	C18H22
SMILES:	CCCCCC(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	238.37
CAS:	1530-04-7

Physical Properties

Property code	Value	Unit	Source
chl	-10230.00	kJ/mol	NIST Webbook
gf	323.06	kJ/mol	Joback Method
hf	52.93	kJ/mol	Joback Method
hfus	26.94	kJ/mol	Joback Method
hvap	59.83	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.399		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
tb	594.18 ± 0.30	K	NIST Webbook
tc	890.11	K	Joback Method
tf	261.39 ± 0.10	K	NIST Webbook
vc	0.822	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.29	J/mol×K	664.16	Joback Method
cpg	663.59	J/mol×K	852.45	Joback Method
cpg	648.97	J/mol×K	814.79	Joback Method
cpg	633.21	J/mol×K	777.13	Joback Method
cpg	616.23	J/mol×K	739.48	Joback Method
cpg	597.96	J/mol×K	701.82	Joback Method
cpg	677.16	J/mol×K	890.11	Joback Method

dvisc	0.0001145	Paxs	664.16	Joback Method
dvisc	0.0001530	Paxs	608.54	Joback Method
dvisc	0.0002169	Paxs	552.93	Joback Method
dvisc	0.0003323	Paxs	497.31	Joback Method
dvisc	0.0005670	Paxs	441.69	Joback Method
dvisc	0.0011284	Paxs	386.08	Joback Method
dvisc	0.0028308	Paxs	330.46	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43785e+01
Coeff. B	-4.76150e+03
Coeff. C	-1.06332e+02
Temperature range (K), min.	444.15
Temperature range (K), max.	631.15

Sources

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=C1530047&Units=SI
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/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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