

1,1-Diphenylcyclopropane

Other names:	Benzene, 1,1'-cyclopropylidenebis-Cyclopropane, 1,1-diphenyl-
Inchi:	InChI=1S/C15H14/c1-3-7-13(8-4-1)15(11-12-15)14-9-5-2-6-10-14/h1-10H,11-12H2
InchiKey:	YHPLHTWUZJURAM-UHFFFAOYSA-N
Formula:	C15H14
SMILES:	<chem>c1ccc(C2(c3ccccc3)CC2)cc1</chem>
Mol. weight [g/mol]:	194.27
CAS:	3282-18-6

Physical Properties

Property code	Value	Unit	Source
chl	-8089.00 ± 3.00	kJ/mol	NIST Webbook
gf	355.50	kJ/mol	Joback Method
hf	208.17	kJ/mol	Joback Method
hfl	185.00 ± 3.00	kJ/mol	NIST Webbook
hfus	14.52	kJ/mol	Joback Method
hvap	52.30	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.767		Crippen Method
mcvol	163.830	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
tb	602.94	K	Joback Method
tc	866.40	K	Joback Method
tf	353.49	K	Joback Method
vc	0.615	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	405.11	J/mol×K	602.94	Joback Method
cpg	423.83	J/mol×K	646.85	Joback Method
cpg	440.96	J/mol×K	690.76	Joback Method
cpg	456.81	J/mol×K	734.67	Joback Method
cpg	471.70	J/mol×K	778.58	Joback Method

cpg	485.93	J/mol×K	822.49	Joback Method
cpg	499.82	J/mol×K	866.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3282186&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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