Benzene, 1,1'-(1,3-propanediyl)bis-

Other names:	1,3-Diphenylpropane
	Propane, 1,3-diphenyl-
Inchi:	InChI=1S/C15H16/c1-3-8-14(9-4-1)12-7-13-15-10-5-2-6-11-15/h1-6,8-11H,7,12-13H2
InchiKey:	VEAFKIYNHVBNIP-UHFFFAOYSA-N
Formula:	C15H16
SMILES:	c1ccc(CCCc2ccccc2)cc1
Mol. weight [g/mol]:	196.29
CAS:	1081-75-0

Physical Properties

Property code	Value	Unit	Source
affp	820.10	kJ/mol	NIST Webbook
basg	787.60	kJ/mol	NIST Webbook
chl	-7887.00	kJ/mol	NIST Webbook
chl	-8245.00	kJ/mol	NIST Webbook
gf	300.24	kJ/mol	Joback Method
hf	120.13	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	53.54	kJ/mol	Joback Method
ie	8.60 ± 0.10	eV	NIST Webbook
ie	8.79 ± 0.05	eV	NIST Webbook
log10ws	-4.31		Crippen Method
logp	3.862		Crippen Method
mcvol	174.690	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	1632.80		NIST Webbook
rinpol	1632.80		NIST Webbook
rinpol	1632.80		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook
ripol	2223.00		NIST Webbook
tb	573.50	K	NIST Webbook
tc	830.66	K	Joback Method
tf	311.65	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.66	J/mol×K	830.66	Joback Method
cpg	421.59	J/mol×K	595.96	Joback Method
cpg	439.86	J/mol×K	635.08	Joback Method
cpg	456.79	J/mol×K	674.19	Joback Method
cpg	472.46	J/mol×K	713.31	Joback Method
cpg	486.94	J/mol×K	752.43	Joback Method
cpg	500.31	J/mol×K	791.54	Joback Method
dvisc	0.0001645	Pa×s	595.96	Joback Method
dvisc	0.0025471	Pa×s	311.65	Joback Method
dvisc	0.0011937	Pa×s	359.04	Joback Method
dvisc	0.0006676	Pa×s	406.42	Joback Method
dvisc	0.0004215	Pa×s	453.81	Joback Method
dvisc	0.0002903	Pa×s	501.19	Joback Method
dvisc	0.0002133	Pa×s	548.58	Joback Method
hvapt	61.50	kJ/mol	459.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	397.20	K	0.30	NIST Webbook
tbrp	441.50 ± 0.50	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45693e+01
Coeff. B	-4.80231e+03
Coeff. C	-9.09030e+01
Temperature range (K), min.	427.16
Temperature range (K), max.	609.63

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1081750&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/ci990307l
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

affp:	Proton affinity
basg:	Gas basicity
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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume