Diphenylacetylene

Other names:	1,1'-(1,2-Ethanediyl)bisbenzene
	1,2-Diphenylacetylene
	1,2-diphenylethyne
	Acetylene, diphenyl-
	Benzene, 1,1'-(1,2-ethynediyl)bis-
	Diphenylethyne
	Ethyne, diphenyl-
	NSC 5185
	Tolan
	Tolane
	biphenylacetylene
Inchi:	InChI=1S/C14H10/c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-14/h1-10H
InchiKey:	JRXXLCKWQFKACW-UHFFFAOYSA-N
Formula:	C14H10
SMILES:	C(#Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	178.23
CAS:	501-65-5

Physical Properties

Property code	Value	Unit	Source
chs	-7250.00 ± 1.00	kJ/mol	NIST Webbook
ea	0.32 ± 0.07	eV	NIST Webbook
gf	494.62	kJ/mol	Joback Method
hf	385.00 ± 2.70	kJ/mol	NIST Webbook
hfus	21.04	kJ/mol	Heat Capacity and Thermodynamic Functions of Diphenylacetylene
hsub	95.10 ± 1.10	kJ/mol	NIST Webbook
hsub	95.30	kJ/mol	NIST Webbook
hvap	53.46	kJ/mol	Joback Method
ie	7.90 ± 0.02	eV	NIST Webbook
ie	7.95 ± 0.08	eV	NIST Webbook
ie	7.94 ± 0.03	eV	NIST Webbook
ie	7.91	eV	NIST Webbook
ie	8.85 ± 0.05	eV	NIST Webbook
ie	23.40 ± 0.10	eV	NIST Webbook
ie	8.00 ± 0.05	eV	NIST Webbook

log10ws	-3.89		Crippen Method
logp	3.086		Crippen Method
mcvol	152.000	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
rinpol	283.20		NIST Webbook
rinpol	291.70		NIST Webbook
rinpol	291.70		NIST Webbook
rinpol	289.27		NIST Webbook
sg	452.00	J/mol×K	NIST Webbook
tb	573.00	K	NIST Webbook
tc	854.17	K	Joback Method
tf	332.15 ± 1.50	K	NIST Webbook
tf	332.15 ± 1.40	K	NIST Webbook
tf	333.00 ± 1.00	K	NIST Webbook
tf	333.00 ± 1.50	K	NIST Webbook
tf	334.75 ± 0.40	K	NIST Webbook
tf	332.15 ± 1.00	K	NIST Webbook
tf	332.20 ± 1.00	K	NIST Webbook
tf	337.00 ± 3.00	K	NIST Webbook
tf	333.80 ± 4.00	K	NIST Webbook
tf	330.00 ± 1.00	K	NIST Webbook
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.38	J/mol×K	854.17	Joback Method
cpg	333.90	J/mol×K	582.08	Joback Method
cpg	404.80	J/mol×K	808.82	Joback Method
cpg	393.16	J/mol×K	763.47	Joback Method
cpg	380.35	J/mol×K	718.13	Joback Method
cpg	366.28	J/mol×K	672.78	Joback Method
cpg	350.83	J/mol×K	627.43	Joback Method
cps	225.90	J/mol×K	298.50	NIST Webbook
cps	297.50	J/mol×K	340.00	NIST Webbook
hfust	20.50	kJ/mol	334.00	NIST Webbook
hfust	21.50	kJ/mol	335.00	NIST Webbook
hfust	20.50	kJ/mol	334.00	NIST Webbook
hsubt	89.00 ± 1.00	kJ/mol	317.00	NIST Webbook
hsubt	88.70 ± 1.30	kJ/mol	310.00	NIST Webbook
hsubt	90.00 ± 4.50	kJ/mol	310.00	NIST Webbook

hvapt	63.80 ± 0.20	kJ/mol	478.00	NIST Webbook
hvapt	58.10 ± 0.30	kJ/mol	478.00	NIST Webbook
hvapt	60.90 ± 0.20	kJ/mol	478.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.00	K	2.50	NIST Webbook
tbrp	443.20	K	2.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	8.02247e+01
Coeff. B	-1.07494e+04
Coeff. C	-9.08276e+00
Coeff. D	2.49180e-06
Temperature range (K), min.	335.65
Temperature range (K), max.	832.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol787.mol
Heat Capacity and Thermodynamic Functions of Diphenylacetylene:	https://www.doi.org/10.1021/je200673a
Vapor-Liquid Equilibrium Behavior of Tolan in Alcohol:	https://www.doi.org/10.1021/je049778g
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C501655&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=787
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	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
sg:	Molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume