Benzene, 1,1'-(1-buten-3-yne-1,4-diyl)bis-

Other names:	Diphenyl-but-3-en-1-yne
	(E)-1,4-Diphenyl-but-3-en-1-yne
Inchi:	InChI=1S/C16H12/c1-3-9-15(10-4-1)13-7-8-14-16-11-5-2-6-12-16/h1-7,9-13H/b13-7+
InchiKey:	LHNRWGOBPNCPKQ-NTUHNPAUSA-N
Formula:	C16H12
SMILES:	C(#Cc1ccccc1)C=Cc1ccccc1
Mol. weight [g/mol]:	204.27
CAS:	13141-45-2

Physical Properties

Property code	Value	Unit	Source
gf	591.68	kJ/mol	Joback Method
hf	489.01	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	57.87	kJ/mol	Joback Method
ie	7.99	eV	NIST Webbook
ie	7.50	eV	NIST Webbook
log10ws	-4.64		Crippen Method
logp	3.752		Crippen Method
mcvol	175.880	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
tb	632.00	K	Joback Method
tc	903.15	K	Joback Method
tf	423.94	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.21	J/mol×K	632.00	Joback Method
cpg	427.70	J/mol×K	677.19	Joback Method
cpg	443.64	J/mol×K	722.38	Joback Method
cpg	458.18	J/mol×K	767.57	Joback Method
cpg	471.44	J/mol×K	812.77	Joback Method

cpg	483.59	J/mol×K	857.96	Joback Method
cpg	494.75	J/mol×K	903.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13141452&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
ie:	Ionization energy
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