

Benzene, 1,1'-ethenylidenebis-

Other names:	1,1-Diphenylethene 1,1-Diphenylethylene NSC 57645 as-Diphenylethylene diphenylethylene unsym-Diphenylethylene «alpha»,«alpha»-Diphenylethylene «alpha»-Methylene-diphenylmethane «alpha»-Phenylstyrene
Inchi:	InChI=1S/C14H12/c1-12(13-8-4-2-5-9-13)14-10-6-3-7-11-14/h2-11H,1H2
InchiKey:	ZMYIIHDQURVDRB-UHFFFAOYSA-N
Formula:	C14H12
SMILES:	C=C(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	180.25
CAS:	530-48-3

Physical Properties

Property code	Value	Unit	Source
af	0.4322		Cheméo Relay (1.0)
affp	885.70	kJ/mol	NIST Webbook
basg	856.90	kJ/mol	NIST Webbook
chl	-7396.50 ± 1.20	kJ/mol	NIST Webbook
ea	0.39 ± 0.06	eV	NIST Webbook
gf	371.11	kJ/mol	Joback Method
hf	303.08	kJ/mol	Cheméo Relay (1.0)
hfus	17.51	kJ/mol	Joback Method
hvap	71.20 ± 0.70	kJ/mol	NIST Webbook
ie	8.00 ± 0.02	eV	NIST Webbook
log10ws	-4.35		Cheméo Relay (1.0)
logp	3.748		Crippen Method
mcvol	156.300	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	289.70		NIST Webbook
rinpol	296.62		NIST Webbook
tb	550.20	K	NIST Webbook
tb	543.70	K	NIST Webbook
tc	804.16	K	Cheméo Relay (1.0)

tf	281.00 ± 4.00	K	NIST Webbook
tf	281.35 ± 0.30	K	NIST Webbook
tf	281.35 ± 0.30	K	NIST Webbook
vc	0.575	m ³ /kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.98	J/mol×K	569.64	Joback Method
cpg	369.36	J/mol×K	611.29	Joback Method
cpg	385.31	J/mol×K	652.94	Joback Method
cpg	399.93	J/mol×K	694.59	Joback Method
cpg	413.31	J/mol×K	736.24	Joback Method
cpg	425.56	J/mol×K	777.89	Joback Method
cpg	436.78	J/mol×K	819.54	Joback Method
cpl	299.20	J/mol×K	298.50	NIST Webbook
hvapt	70.20 ± 0.70	kJ/mol	314.50	NIST Webbook
hvapt	59.30	kJ/mol	455.00	NIST Webbook
hvapt	73.30	kJ/mol	512.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46567e+01
Coeff. B	-4.51305e+03
Coeff. C	-9.41190e+01
Temperature range (K), min.	408.20
Temperature range (K), max.	577.05

Sources

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

**The Yaws Handbook of Vapor
Pressure:
NIST Webbook:**

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C530483&Units=SI>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

af:	Acentric Factor
affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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