

Benzene, 1,1',1'',1'''-(1,2-ethenediylidene)tetrakis-

Other names:

1,1,2,2-TETRAPHENYLETHYLENE

1,1,2,2-Tetraphenylethene

Ethylene, tetraphenyl-

TETRAPHENYLETHYLENE

Tetraphenylethene

«alpha», «beta»-Diphenylstilbene

Â«alphaÂ»,Â«betaÂ»-Diphenylstilbene

Inchi: InChI=1S/C26H20/c1-5-13-21(14-6-1)25(22-15-7-2-8-16-22)26(23-17-9-3-10-18-23)24-1

InchiKey: JLZUZNKTTIRERF-UHFFFAOYSA-N

Formula: C26H20

SMILES: c1ccc(C(=C(c2ccccc2)c2ccccc2)c2ccccc2)cc1

Mol. weight [g/mol]: 332.44

CAS: 632-51-9

Physical Properties

Property code	Value	Unit	Source
chs	-13401.10 ± 1.30	kJ/mol	NIST Webbook
gf	680.80	kJ/mol	Joback Method
hf	463.79	kJ/mol	Joback Method
hfus	36.84	kJ/mol	Joback Method
hsub	133.40 ± 0.70	kJ/mol	NIST Webbook
hvap	82.69	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	6.694		Crippen Method
mcvol	277.860	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	2478.00		NIST Webbook
rinpol	2478.00		NIST Webbook
rinpol	2478.00		NIST Webbook
rinpol	2478.00		NIST Webbook
tb	693.20	K	NIST Webbook
tc	1190.36	K	Joback Method
tf	495.00 ± 3.00	K	NIST Webbook
tf	497.90 ± 0.40	K	NIST Webbook
tf	497.85 ± 0.30	K	NIST Webbook
tf	500.00 ± 2.00	K	NIST Webbook
tf	497.00 ± 1.50	K	NIST Webbook

tf	494.00 ± 3.00	K	NIST Webbook
tf	494.40 ± 1.50	K	NIST Webbook
tf	494.40 ± 1.50	K	NIST Webbook
tf	499.20 ± 4.00	K	NIST Webbook
vc	1.042	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	897.94	J/mol×K	1142.78	Joback Method
cpg	822.01	J/mol×K	904.92	Joback Method
cpg	839.46	J/mol×K	952.49	Joback Method
cpg	855.49	J/mol×K	1000.07	Joback Method
cpg	870.39	J/mol×K	1047.64	Joback Method
cpg	884.44	J/mol×K	1095.21	Joback Method
cpg	911.19	J/mol×K	1190.36	Joback Method
cps	387.60	J/mol×K	298.50	NIST Webbook
hfust	37.45	kJ/mol	496.10	NIST Webbook
hsubt	129.30 ± 0.70	kJ/mol	366.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.32254e+01
Coeff. B	-1.01474e+04
Coeff. C	-1.32355e+02
Temperature range (K), min.	574.74
Temperature range (K), max.	698.81

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/T + C \cdot \ln(T) + D \cdot T^2$
Coeff. A	1.40520e+02
Coeff. B	-1.95081e+04
Coeff. C	-1.68964e+01

Coeff. D	3.17740e-06
Temperature range (K), min.	496.15
Temperature range (K), max.	996.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=816
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C632519&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.therc.org/research/kdb/hcprop/showprop.php?cmpid=816
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
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
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

Latest version available from:

<https://www.cheméo.com/cid/63-984-0/Benzene-1-1-1-1-2-ethenediylidene-tetrakis.pdf>

Generated by Cheméo on 2024-04-20 09:30:44.18126398 +0000 UTC m=+15894693.101841293.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.