

1,1,1,2-Tetraphenylethane

Other names: Benzene, 1,1',1'',1'''-(1-ethanyl-2-ylidyne)tetrakis-

Ethane, 1,1,1,2-tetraphenyl-

Inchi: InChI=1S/C26H22/c1-5-13-22(14-6-1)21-26(23-15-7-2-8-16-23,24-17-9-3-10-18-24)25-19

InchiKey: KGSFMPRFQVLGTJ-UHFFFAOYSA-N

Formula: C26H22

SMILES: c1ccc(CC(c2ccccc2)(c2ccccc2)c2ccccc2)cc1

Mol. weight [g/mol]: 334.45

CAS: 2294-94-2

Physical Properties

Property code	Value	Unit	Source
chs	-13401.10 ± 1.30	kJ/mol	NIST Webbook
chs	-13606.00 ± 3.00	kJ/mol	NIST Webbook
gf	620.52	kJ/mol	Joback Method
hf	365.00 ± 3.00	kJ/mol	NIST Webbook
hfs	233.00 ± 3.00	kJ/mol	NIST Webbook
hfus	31.85	kJ/mol	Joback Method
hsub	133.00	kJ/mol	NIST Webbook
hsub	132.60 ± 2.10	kJ/mol	NIST Webbook
hsub	132.00	kJ/mol	NIST Webbook
hvap	81.28	kJ/mol	Joback Method
log10ws	-7.00		Crippen Method
logp	6.264		Crippen Method
mcvol	282.160	ml/mol	McGowan Method
pc	1778.84	kPa	Joback Method
tb	897.77	K	Joback Method
tc	1179.33	K	Joback Method
tf	414.25 ± 0.50	K	NIST Webbook
tf	416.75 ± 0.30	K	NIST Webbook
tf	417.00 ± 2.00	K	NIST Webbook
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.52	J/molxK	1179.33	Joback Method
cpg	927.56	J/molxK	1132.41	Joback Method
cpg	914.23	J/molxK	1085.48	Joback Method
cpg	900.25	J/molxK	1038.55	Joback Method
cpg	885.31	J/molxK	991.62	Joback Method
cpg	869.13	J/molxK	944.70	Joback Method
cpg	851.41	J/molxK	897.77	Joback Method
cps	395.40	J/molxK	298.50	NIST Webbook
dvisc	0.0000378	Paxs	897.77	Joback Method
dvisc	0.0006814	Paxs	490.88	Joback Method
dvisc	0.0000502	Paxs	829.95	Joback Method
dvisc	0.0000703	Paxs	762.14	Joback Method
dvisc	0.0001050	Paxs	694.33	Joback Method
dvisc	0.0001711	Paxs	626.51	Joback Method
dvisc	0.0003140	Paxs	558.69	Joback Method
hsubt	128.70 ± 2.10	kJ/mol	370.00	NIST Webbook
hsubt	126.40 ± 1.70	kJ/mol	434.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	551.70	K	2.80	NIST Webbook

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2294942&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

Joback Method:

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

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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