

Benzene, 1,1',1'',1'''-(1,3-butadiene-1,4-diylidene)tetrakis-

Other names:

1,3-Butadiene, 1,1,4,4-tetraphenyl-

1,1,4,4-Tetraphenyl-1,3-butadiene

1,1,4,4-Tetraphenylbutadiene

1,1,4,4-tetraphenylbuta-1,3-diene

Inchi:

InChI=1S/C28H22/c1-5-13-23(14-6-1)27(24-15-7-2-8-16-24)21-22-28(25-17-9-3-10-18-2)

InchiKey:

KLCLIOISYBHYDZ-UHFFFAOYSA-N

Formula:

C₂₈H₂₂

SMILES:

C(C=C(c1ccccc1)c1ccccc1)=C(c1ccccc1)c1ccccc1

Mol. weight [g/mol]:

358.47

CAS:

1450-63-1

Physical Properties

Property code	Value	Unit	Source
chs	-14492.30 ± 3.00	kJ/mol	NIST Webbook
gf	777.86	kJ/mol	Joback Method
hf	539.73	kJ/mol	Joback Method
hfus	42.22	kJ/mol	Joback Method
hvap	87.10	kJ/mol	Joback Method
log10ws	-8.20		Crippen Method
logp	7.250		Crippen Method
mcvol	301.740	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
tb	954.84	K	Joback Method
tc	1237.13	K	Joback Method
tf	472.92	K	Joback Method
vc	1.133	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.19	J/mol×K	954.84	Joback Method
cpg	928.75	J/mol×K	1001.89	Joback Method
cpg	945.32	J/mol×K	1048.94	Joback Method
cpg	961.20	J/mol×K	1095.98	Joback Method

cpg	976.74	J/mol×K	1143.03	Joback Method
cpg	992.26	J/mol×K	1190.08	Joback Method
cpg	1008.08	J/mol×K	1237.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1450631&Units=SI
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

Legend

chs:	Standard solid enthalpy of combustion
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
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

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