

Benzene, 1,1',1'',1'''-(1,4-butanediylidene)tetrakis-

Other names:

1,1,4,4-Tetraphenylbutane

Inchi: InChI=1S/C28H26/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: RYRPAXUFKAJVQC-UHFFFAOYSA-N

Formula: C28H26

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

Mol. weight [g/mol]: 362.51

CAS: 1483-64-3

Physical Properties

Property code	Value	Unit	Source
chs	-14897.30 ± 4.00	kJ/mol	NIST Webbook
gf	629.64	kJ/mol	Joback Method
hf	314.31	kJ/mol	Joback Method
hfus	37.39	kJ/mol	Joback Method
hvap	86.25	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	7.431		Crippen Method
mcvol	310.340	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
tb	945.88	K	Joback Method
tc	1211.98	K	Joback Method
tf	481.00	K	Joback Method
vc	1.159	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	969.82	J/mol×K	945.88	Joback Method
cpg	987.22	J/mol×K	990.23	Joback Method
cpg	1003.16	J/mol×K	1034.58	Joback Method
cpg	1017.84	J/mol×K	1078.93	Joback Method
cpg	1031.49	J/mol×K	1123.28	Joback Method
cpg	1044.34	J/mol×K	1167.63	Joback Method
cpg	1056.60	J/mol×K	1211.98	Joback Method

dvisc	0.0007746	Paxs	481.00	Joback Method
dvisc	0.0003117	Paxs	558.48	Joback Method
dvisc	0.0001566	Paxs	635.96	Joback Method
dvisc	0.0000913	Paxs	713.44	Joback Method
dvisc	0.0000592	Paxs	790.92	Joback Method
dvisc	0.0000415	Paxs	868.40	Joback Method
dvisc	0.0000308	Paxs	945.88	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1483643&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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