

Benzene, 1,1',1'',1''',1'''',1'''''-(1,2-ethanediylidyne)hexakis-

Other names:

Hexaphenylethane

Ethane, hexaphenyl-

Inchi:

InChI=1S/C38H30/c1-6-16-30(17-7-1)37(31-18-8-2-9-19-31)32-26-28-36(29-27-32)38(33

InchiKey:

IYDPHZDMGCHZFB-UHFFFAOYSA-N

Formula:

C38H30

SMILES:

C1=CC(=C(c2ccccc2)c2ccccc2)CC=C1C(c1ccccc1)(c1ccccc1)c1ccccc1

Mol. weight [g/mol]:

486.64

CAS:

17854-07-8

Physical Properties

Property code	Value	Unit	Source
chs	-19920.00	kJ/mol	NIST Webbook
gf	953.33	kJ/mol	Joback Method
hf	591.24	kJ/mol	Joback Method
hfs	619.20	kJ/mol	NIST Webbook
hfus	48.80	kJ/mol	Joback Method
hvap	113.12	kJ/mol	Joback Method
log10ws	-10.85		Crippen Method
logp	9.409		Crippen Method
mcvol	403.720	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
tb	1233.05	K	Joback Method
tc	1538.75	K	Joback Method
tf	674.60	K	Joback Method
vc	1.502	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1362.82	J/molxK	1233.05	Joback Method
cpg	1383.03	J/molxK	1284.00	Joback Method
cpg	1404.13	J/molxK	1334.95	Joback Method
cpg	1426.66	J/molxK	1385.90	Joback Method
cpg	1451.15	J/molxK	1436.85	Joback Method

cpg	1478.12	J/mol×K	1487.80	Joback Method
cpg	1508.09	J/mol×K	1538.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17854078&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
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
hfs:	Solid phase 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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