Benzene, 1,1',1'',1''',1'''',1'''''-[bi-2-cyclopropen-1-yl]-1,1',2,2',

Other names: Cyclopropene,bis-3,3'-triphenyl-

Inchi: InChI=1S/C42H30/c1-7-19-31(20-8-1)37-38(32-21-9-2-10-22-32)41(37,35-27-15-5-16-28

InchiKey: DQELQSOUCKXCIO-UHFFFAOYSA-N

Formula: C42H30

SMILES: c1ccc(C2=C(c3ccccc3)C2(c2ccccc2)C2(c3ccccc3)C(c3ccccc3)=C2c2ccccc2)cc1

Mol. weight [g/mol]: 534.69

CAS: 4997-62-0

Physical Properties

Property code	Value	Unit	Source
gf	1109.14	kJ/mol	Joback Method
hf	754.73	kJ/mol	Joback Method
hfus	53.34	kJ/mol	Joback Method
hvap	123.50	kJ/mol	Joback Method
ie	7.72 ± 0.05	eV	NIST Webbook
log10ws	-11.53		Crippen Method
logp	10.112		Crippen Method
mcvol	429.760	ml/mol	McGowan Method
pc	1187.42	kPa	Joback Method
tb	1352.64	K	Joback Method
tc	1670.82	K	Joback Method
tf	856.90	K	Joback Method
vc	1.621	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1751.70	J/mol×K	1352.64	Joback Method
cpg	1838.45	J/mol×K	1405.67	Joback Method
cpg	1936.52	J/mol×K	1458.70	Joback Method
cpg	2047.10	J/mol×K	1511.73	Joback Method
cpg	2171.40	J/mol×K	1564.76	Joback Method
cpg	2310.63	J/mol×K	1617.79	Joback Method
cpg	2465.99	J/mol×K	1670.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4997620&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

Legend

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
ie:	Ionization energy
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