7,7'-bis(Cycloheptatrienyl)

Other names: Bicycloheptatrienyl
Inchi: InChI=1S/C14H14/c1-2-6-10-13(9-5-1)14-11-7-3-4-8-12-14/h1-14H
InchiKey: DMVKBMNNLFFZBY-UHFFFAOYSA-N
Formula: C14H14
SMILES: C1=CC=CC(C2C=CC=CC=C2)C=C1
Mol. weight [g/mol]: 182.26
CAS: 39473-62-6

Physical Properties

Property code	Value	Unit	Source
gf	271.46	kJ/mol	Joback Method
hf	110.71	kJ/mol	Joback Method
hfus	18.82	kJ/mol	Joback Method
hvap	49.71	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
ie	8.62	eV	NIST Webbook
log10ws	-4.11		Crippen Method
logp	3.583		Crippen Method
mcvol	160.600	ml/mol	McGowan Method
pc	2811.36	kPa	Joback Method
tb	562.32	K	Joback Method
tc	818.01	K	Joback Method
tf	259.82	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.84	J/mol×K	562.32	Joback Method
cpg	469.50	J/mol×K	775.40	Joback Method
cpg	454.17	J/mol×K	732.78	Joback Method
cpg	437.31	J/mol×K	690.17	Joback Method
cpg	418.84	J/mol×K	647.55	Joback Method
cpg	398.71	J/mol×K	604.94	Joback Method

cpg	483.36	J/mol×K	818.01	Joback Method
dvisc	0.0001444	Pa×s	562.32	Joback Method
dvisc	0.0001955	Pa×s	511.90	Joback Method
dvisc	0.0002827	Pa×s	461.49	Joback Method
dvisc	0.0004477	Pa×s	411.07	Joback Method
dvisc	0.0008061	Pa×s	360.65	Joback Method
dvisc	0.0017571	Pa×s	310.24	Joback Method
dvisc	0.0051829	Pa×s	259.82	Joback Method

Sources

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=C39473626&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.