1,2-Cyclobuta-3,4:5,6 bicyclopentabenzene

Other names: 1,2-Cyclobuteno-3,4:5,6-bi(cyclopenteno)benzene
Inchi: InChI=1S/C14H16/c1-3-9-10-4-2-6-12(10)14-8-7-13(14)11(9)5-1/h1-8H2
InchiKey: LWTCAZSEGNGWRU-UHFFFAOYSA-N
Formula: C14H16
SMILES: C1Cc2c3c(c4c(c2C1)CC4)CCC3
Mol. weight [g/mol]: 184.28
CAS: 54922-12-2

Physical Properties

Property code	Value	Unit	Source
gf	348.74	kJ/mol	Joback Method
hf	132.47	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	52.84	kJ/mol	Joback Method
ie	7.95 ± 0.05	eV	NIST Webbook
log10ws	-4.30		Crippen Method
logp	2.763		Crippen Method
mcvol	151.780	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
tb	601.26	K	Joback Method
tc	839.15	K	Joback Method
tf	406.62	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.14	J/mol×K	601.26	Joback Method
cpg	411.73	J/mol×K	640.91	Joback Method
cpg	427.04	J/mol×K	680.56	Joback Method
cpg	441.26	J/mol×K	720.21	Joback Method
cpg	454.54	J/mol×K	759.86	Joback Method
cpg	467.08	J/mol×K	799.50	Joback Method
cpg	479.05	J/mol×K	839.15	Joback Method

dvisc	0.0026232	Pa×s	406.62	Joback Method
dvisc	0.0024446	Pa×s	439.06	Joback Method
dvisc	0.0023004	Pa×s	471.50	Joback Method
dvisc	0.0021817	Pa×s	503.94	Joback Method
dvisc	0.0020825	Pa×s	536.38	Joback Method
dvisc	0.0019983	Pa×s	568.82	Joback Method
dvisc	0.0019261	Pa×s	601.26	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=C54922122&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