[2.2.2](1,2,4)Cyclophane

Inchi: InChI=1S/C18H18/c1-2-14-4-6-16-8-7-15-5-3-13(1)11-17(15)9-10-18(16)12-14/h3-6,11-1
InchiKey: APDVWYTWRPQAFD-UHFFFAOYSA-N
Formula: C18H18
SMILES: c1cc2c3cc1CCc1ccc(c(c1)CC3)CC2
Mol. weight [g/mol]: 234.34
CAS: 58002-98-5

Physical Properties

Property code	Value	Unit	Source
gf	423.90	kJ/mol	Joback Method
hf	198.61	kJ/mol	Joback Method
hfus	23.03	kJ/mol	Joback Method
hvap	63.31	kJ/mol	Joback Method
ie	8.00 ± 0.10	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-5.22		Crippen Method
logp	3.669		Crippen Method
mcvol	195.240	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
tb	707.34	K	Joback Method
tc	963.48	K	Joback Method
tf	439.90	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.83	J/mol×K	707.34	Joback Method
cpg	559.16	J/mol×K	750.03	Joback Method
cpg	576.10	J/mol×K	792.72	Joback Method
cpg	591.85	J/mol×K	835.41	Joback Method
cpg	606.60	J/mol×K	878.10	Joback Method
cpg	620.54	J/mol×K	920.79	Joback Method
cpg	633.86	J/mol×K	963.48	Joback Method

dvisc	0.0019344	Pa×s	439.90	Joback Method
dvisc	0.0014644	Pa×s	484.47	Joback Method
dvisc	0.0011619	Pa×s	529.05	Joback Method
dvisc	0.0009556	Pa×s	573.62	Joback Method
dvisc	0.0008084	Pa×s	618.19	Joback Method
dvisc	0.0006994	Pa×s	662.77	Joback Method
dvisc	0.0006163	Pa×s	707.34	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=C58002985&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