2-Methyl[2.2]paracyclophane

Inchi: InChI=1S/C17H18/c1-13-12-16-7-6-14-2-4-15(5-3-14)8-10-17(13)11-9-16/h2-5,9,11-12H,
InchiKey: PCWILLLONPHNNY-UHFFFAOYSA-N
Formula: C17H18
SMILES: Cc1cc2ccc1CCc1ccc(cc1)CC2
Mol. weight [g/mol]: 222.32
CAS: 24262-07-5

Physical Properties

Property code	Value	Unit	Source
gf	344.55	kJ/mol	Joback Method
hf	131.42	kJ/mol	Joback Method
hfus	21.67	kJ/mol	Joback Method
hvap	60.37	kJ/mol	Joback Method
ie	7.60	eV	NIST Webbook
ie	7.90 ± 0.05	eV	NIST Webbook
log10ws	-5.03		Crippen Method
logp	3.879		Crippen Method
mcvol	192.010	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
tb	672.34	K	Joback Method
tc	924.68	K	Joback Method
tf	390.41	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.68	J/mol×K	672.34	Joback Method
cpg	527.93	J/mol×K	714.40	Joback Method
cpg	545.68	J/mol×K	756.45	Joback Method
cpg	562.05	J/mol×K	798.51	Joback Method
cpg	577.16	J/mol×K	840.57	Joback Method
cpg	591.13	J/mol×K	882.62	Joback Method
cpg	604.07	J/mol×K	924.68	Joback Method

dvisc	0.0014582	Pa×s	390.41	Joback Method
dvisc	0.0008961	Pa×s	437.40	Joback Method
dvisc	0.0006052	Pa×s	484.39	Joback Method
dvisc	0.0004382	Pa×s	531.38	Joback Method
dvisc	0.0003343	Pa×s	578.36	Joback Method
dvisc	0.0002657	Pa×s	625.35	Joback Method
dvisc	0.0002180	Pa×s	672.34	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=C24262075&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