

Pentacyclo[10.2.2.2^{5,8}.0^{2,4}

Other names:	7,8:7',8'-bismethano-[2.2]paracyclophane Pentacyclo[10.2.2.2
Inchi:	InChI=1S/C18H16/c1-2-12-4-3-11(1)15-9-17(15)13-5-7-14(8-6-13)18-10-16(12)18/h1-8,1
InchiKey:	DOPCIYVVYMITKB-UHFFFAOYSA-N
Formula:	C18H16
SMILES:	c1cc2ccc1C1CC1c1ccc(cc1)C1CC21
Mol. weight [g/mol]:	232.32
CAS:	83944-24-5

Physical Properties

Property code	Value	Unit	Source
gf	517.08	kJ/mol	Joback Method
hf	251.81	kJ/mol	Joback Method
hfus	31.46	kJ/mol	Joback Method
hvap	60.45	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.542		Crippen Method
mvol	184.380	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
tb	677.30	K	Joback Method
tc	925.04	K	Joback Method
tf	430.64	K	Joback Method
vc	0.722	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.58	J/molxK	677.30	Joback Method
cpg	607.37	J/molxK	883.75	Joback Method
cpg	593.28	J/molxK	842.46	Joback Method
cpg	578.49	J/molxK	801.17	Joback Method
cpg	562.77	J/molxK	759.88	Joback Method
cpg	545.88	J/molxK	718.59	Joback Method
cpg	621.01	J/molxK	925.04	Joback Method

dvisc	0.0067284	Paxs	677.30	Joback Method
dvisc	0.0064360	Paxs	636.19	Joback Method
dvisc	0.0061187	Paxs	595.08	Joback Method
dvisc	0.0057735	Paxs	553.97	Joback Method
dvisc	0.0053973	Paxs	512.86	Joback Method
dvisc	0.0049866	Paxs	471.75	Joback Method
dvisc	0.0045382	Paxs	430.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83944245&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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

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