Pentacyclo[10.2.2.25,8.02,4.09,11]octadeca-5,7,12

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]: 232.33

Physical Properties

Property code	Value	Unit	Source
hfus	31.46	kJ/mol	Joback Method
ie	7.40	eV	NIST Webbook
ie	7.90	eV	NIST Webbook
logp	4.542		Crippen Method
mcvol	184.380	ml/mol	McGowan Method
tb	627.13	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.58	J/mol×K	677.30	Joback Method
cpg	545.88	J/mol×K	718.59	Joback Method
cpg	562.77	J/mol×K	759.88	Joback Method
cpg	578.49	J/mol×K	801.17	Joback Method
cpg	593.28	J/mol×K	842.46	Joback Method
cpg	607.37	J/mol×K	883.75	Joback Method
cpg	621.01	J/mol×K	925.04	Joback Method
dvisc	0.0045382	Pa×s	430.64	Joback Method
dvisc	0.0049866	Pa×s	471.75	Joback Method
dvisc	0.0053973	Pa×s	512.86	Joback Method
dvisc	0.0057735	Pa×s	553.97	Joback Method
dvisc	0.0061187	Pa×s	595.08	Joback Method
dvisc	0.0064360	Pa×s	636.19	Joback Method
dvisc	0.0067284	Pa×s	677.30	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C83944245&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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