1,2,4,5-1',2',4',5'-[2.2.2.2]Cyclooctatetraenocyclop

Inchi: InChI=1S/C22H22/c1-2-16-6-10-20-13-19-9-5-15(1)17-3-4-18(16)8-12-22(20)14-21(19)1
InchiKey: PNGMPACZUFTVCX-JBVUJCTDSA-N
Formula: C22H22
SMILES: C1=CC2=C3C=CC4=C1CCc1cc(c(cc1CC4)CC3)CC2
Mol. weight [g/mol]: 286.41
CAS: 84954-89-2

Physical Properties

Property code	Value	Unit	Source
gf	524.64	kJ/mol	Joback Method
hf	237.87	kJ/mol	Joback Method
hfus	28.80	kJ/mol	Joback Method
hvap	74.22	kJ/mol	Joback Method
ie	7.35	eV	NIST Webbook
log10ws	-7.03		Crippen Method
logp	5.177		Crippen Method
mcvol	236.440	ml/mol	McGowan Method
pc	2051.17	kPa	Joback Method
tb	823.66	K	Joback Method
tc	1084.14	K	Joback Method
tf	529.44	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	718.25	J/mol×K	823.66	Joback Method
cpg	736.94	J/mol×K	867.07	Joback Method
cpg	754.59	J/mol×K	910.49	Joback Method
cpg	771.44	J/mol×K	953.90	Joback Method
cpg	787.75	J/mol×K	997.32	Joback Method
cpg	803.77	J/mol×K	1040.73	Joback Method
cpg	819.74	J/mol×K	1084.14	Joback Method
dvisc	0.0022485	Pa×s	529.44	Joback Method

dvisc	0.0017814	Pa×s	578.48	Joback Method
dvisc	0.0014636	Pa×s	627.51	Joback Method
dvisc	0.0012373	Pa×s	676.55	Joback Method
dvisc	0.0010700	Pa×s	725.59	Joback Method
dvisc	0.0009425	Pa×s	774.62	Joback Method
dvisc	0.0008428	Pa×s	823.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84954892&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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