

[2.2.2.2](1,2,3,5)Cyclophane

Inchi:	InChI=1S/C20H20/c1-2-14-11-17-5-3-15-9-13(1)10-16-4-6-18(12-14)20(17)8-7-19(15)16
InchiKey:	WHLLKTALFBGZGG-UHFFFAOYSA-N
Formula:	C20H20
SMILES:	<chem>c1c2cc3c4c1CCc1cc(cc(c1CC4)CC3)CC2</chem>
Mol. weight [g/mol]:	260.37
CAS:	61477-04-1

Physical Properties

Property code	Value	Unit	Source
gf	502.04	kJ/mol	Joback Method
hf	233.69	kJ/mol	Joback Method
hfus	26.60	kJ/mol	Joback Method
hvap	69.13	kJ/mol	Joback Method
ie	7.75 ± 0.02	eV	NIST Webbook
log10ws	-5.88		Crippen Method
logp	3.768		Crippen Method
mcvol	212.560	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
tb	770.20	K	Joback Method
tc	1024.71	K	Joback Method
tf	513.18	K	Joback Method
vc	0.822	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.77	J/mol×K	770.20	Joback Method
cpg	706.97	J/mol×K	982.29	Joback Method
cpg	691.75	J/mol×K	939.87	Joback Method
cpg	676.27	J/mol×K	897.45	Joback Method
cpg	660.28	J/mol×K	855.04	Joback Method
cpg	643.53	J/mol×K	812.62	Joback Method
cpg	722.18	J/mol×K	1024.71	Joback Method
dvisc	0.0017968	Paxs	770.20	Joback Method

dvisc	0.0019300	Paxs	727.36	Joback Method
dvisc	0.0020916	Paxs	684.53	Joback Method
dvisc	0.0022914	Paxs	641.69	Joback Method
dvisc	0.0025431	Paxs	598.85	Joback Method
dvisc	0.0028682	Paxs	556.02	Joback Method
dvisc	0.0033005	Paxs	513.18	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C61477041&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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