

2,5,3',6'-Tetramethyl-[2.2]paracyclophane

Inchi:	InChI=1S/C20H24/c1-13-9-18-7-8-20-12-15(3)19(11-16(20)4)6-5-17(13)10-14(18)2/h9-12
InchiKey:	JTMLLDPOLFRPGJ-UHFFFAOYSA-N
Formula:	C20H24
SMILES:	<chem>Cc1cc2c(C)cc1CCc1cc(C)c(cc1C)CC2</chem>
Mol. weight [g/mol]:	264.40
CAS:	35233-72-8

Physical Properties

Property code	Value	Unit	Source
gf	340.92	kJ/mol	Joback Method
hf	35.09	kJ/mol	Joback Method
hfus	28.27	kJ/mol	Joback Method
hvap	69.03	kJ/mol	Joback Method
ie	7.55 ± 0.05	eV	NIST Webbook
log10ws	-6.46		Crippen Method
logp	4.804		Crippen Method
mcvol	234.280	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
tb	755.92	K	Joback Method
tc	994.98	K	Joback Method
tf	461.78	K	Joback Method
vc	0.889	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.01	J/molxK	755.92	Joback Method
cpg	690.35	J/molxK	795.76	Joback Method
cpg	708.38	J/molxK	835.61	Joback Method
cpg	725.18	J/molxK	875.45	Joback Method
cpg	740.83	J/molxK	915.29	Joback Method
cpg	755.43	J/molxK	955.14	Joback Method
cpg	769.06	J/molxK	994.98	Joback Method
dvisc	0.0008301	Paxs	461.78	Joback Method

dvisc	0.0005595	Paxs	510.80	Joback Method
dvisc	0.0004041	Paxs	559.83	Joback Method
dvisc	0.0003075	Paxs	608.85	Joback Method
dvisc	0.0002438	Paxs	657.87	Joback Method
dvisc	0.0001996	Paxs	706.90	Joback Method
dvisc	0.0001677	Paxs	755.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C35233728&Units=SI

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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