Tricyclo[8.2.2.2^{4,7}]hexadeca-4,6,10,1

Other names:	2,5,2',5'-Tetramethyl-[2.2]paracyclophane
	Tricyclo[8.2.2.2
Inchi:	InChI=1S/C20H24/c1-13-9-17-5-6-18-11-15(3)20(16(4)12-18)8-7-19(13)14(2)10-17/h9-12
InchiKey:	LBFPZAXQCRQAOQ-UHFFFAOYSA-N
Formula:	C20H24
SMILES:	Cc1cc2cc(C)c1CCc1c(C)cc(cc1C)CC2
Mol. weight [g/mol]:	264.40
CAS:	35233-71-7

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	7.20	eV	NIST Webbook
ie	7.75 ± 0.05	eV	NIST Webbook
ie	7.52	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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.01	J/mol×K	755.92	Joback Method
cpg	690.35	J/mol×K	795.76	Joback Method
cpg	708.38	J/mol×K	835.61	Joback Method
cpg	725.18	J/mol×K	875.45	Joback Method

cpg	740.83	J/mol×K	915.29	Joback Method
cpg	755.43	J/mol×K	955.14	Joback Method
cpg	769.06	J/mol×K	994.98	Joback Method
dvisc	0.0008301	Pa×s	461.78	Joback Method
dvisc	0.0005595	Pa×s	510.80	Joback Method
dvisc	0.0004041	Pa×s	559.83	Joback Method
dvisc	0.0003075	Pa×s	608.85	Joback Method
dvisc	0.0002438	Pa×s	657.87	Joback Method
dvisc	0.0001996	Pa×s	706.90	Joback Method
dvisc	0.0001677	Pa×s	755.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35233717&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

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