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

Inchi: InChI=1S/C16H20/c1-2-14-4-3-13(1)9-10-15-5-7-16(8-6-15)12-11-14/h1,4-5,8H,2-3,6-7,9
InchiKey: SOYXMIFOQRQXKU-UHFFFAOYSA-N
Formula: C16H20
SMILES: C1=C2CC=C(C1)CCC1=CCC(=CC1)CC2
Mol. weight [g/mol]: 212.33
CAS: 26050-79-3

Physical Properties

Property code	Value	Unit	Source
gf	285.84	kJ/mol	Joback Method
hf	47.97	kJ/mol	Joback Method
hfus	17.02	kJ/mol	Joback Method
hvap	56.90	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
log10ws	-5.62		Crippen Method
logp	4.854		Crippen Method
mcvol	186.520	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
tb	646.16	K	Joback Method
tc	898.51	K	Joback Method
tf	365.10	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.70	J/mol×K	646.16	Joback Method
cpg	523.28	J/mol×K	688.22	Joback Method
cpg	543.19	J/mol×K	730.28	Joback Method
cpg	561.54	J/mol×K	772.33	Joback Method
cpg	578.46	J/mol×K	814.39	Joback Method
cpg	594.07	J/mol×K	856.45	Joback Method
cpg	608.49	J/mol×K	898.51	Joback Method

dvisc	0.0021672	Pa×s	365.10	Joback Method
dvisc	0.0011925	Pa×s	411.94	Joback Method
dvisc	0.0007413	Pa×s	458.79	Joback Method
dvisc	0.0005032	Pa×s	505.63	Joback Method
dvisc	0.0003648	Pa×s	552.47	Joback Method
dvisc	0.0002781	Pa×s	599.32	Joback Method
dvisc	0.0002205	Pa×s	646.16	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=C26050793&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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