1,2,3,4,5,6-Hexahydro[2.2]paracyclophane

Inchi: InChI=1S/C16H24/c1-2-14-4-3-13(1)9-10-15-5-7-16(8-6-15)12-11-14/h1,4,15-16H,2-3,5-
InchiKey: JTUHZHSIIGRXJX-UHFFFAOYSA-N
Formula: C16H24
SMILES: C1=C2CC=C(C1)CCC1CCC(CC2)CC1
Mol. weight [g/mol]: 216.36
CAS: 90817-44-0

Physical Properties

Property code	Value	Unit	Source
gf	229.76	kJ/mol	Joback Method
hf	-85.33	kJ/mol	Joback Method
hfus	17.50	kJ/mol	Joback Method
hvap	54.37	kJ/mol	Joback Method
ie	8.00	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
log10ws	-5.43		Crippen Method
logp	5.013		Crippen Method
mcvol	195.120	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
tb	628.54	K	Joback Method
tc	874.46	K	Joback Method
tf	330.06	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.76	J/mol×K	628.54	Joback Method
cpg	574.45	J/mol×K	669.53	Joback Method
cpg	598.25	J/mol×K	710.51	Joback Method
cpg	620.24	J/mol×K	751.50	Joback Method
cpg	640.54	J/mol×K	792.49	Joback Method
cpg	659.25	J/mol×K	833.47	Joback Method
cpg	676.48	J/mol×K	874.46	Joback Method

dvisc	0.0034075	Pa×s	330.06	Joback Method
dvisc	0.0017241	Pa×s	379.81	Joback Method
dvisc	0.0010215	Pa×s	429.55	Joback Method
dvisc	0.0006747	Pa×s	479.30	Joback Method
dvisc	0.0004817	Pa×s	529.05	Joback Method
dvisc	0.0003645	Pa×s	578.79	Joback Method
dvisc	0.0002882	Pa×s	628.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90817440&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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