6,6-Paracyclophane

Inchi: InChI=1S/C24H32/c1-2-6-10-22-17-19-24(20-18-22)12-8-4-3-7-11-23-15-13-21(9-5-1)14-
InchiKey: KZCIQXIXTWAXSA-UHFFFAOYSA-N
Formula: C24H32
SMILES: c1cc2ccc1CCCCCCc1ccc(cc1)CCCCCC2
Mol. weight [g/mol]: 320.51
CAS: 4384-23-0

Physical Properties

Property code	Value	Unit	Source
chs	-13825.00 ± 9.60	kJ/mol	NIST Webbook
gf	316.32	kJ/mol	Joback Method
hf	-77.00 ± 12.00	kJ/mol	NIST Webbook
hfs	-192.00 ± 9.60	kJ/mol	NIST Webbook
hfus	23.38	kJ/mol	Joback Method
hsub	115.00	kJ/mol	NIST Webbook
hsub	115.00 ± 2.00	kJ/mol	NIST Webbook
hsub	115.10 ± 2.10	kJ/mol	NIST Webbook
hvap	76.66	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	6.691		Crippen Method
mcvol	290.640	ml/mol	McGowan Method
pc	1597.44	kPa	Joback Method
tb	861.68	K	Joback Method
tc	1134.76	K	Joback Method
tf	428.62	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	940.06	J/mol×K	861.68	Joback Method
cpg	963.87	J/mol×K	907.19	Joback Method
cpg	984.76	J/mol×K	952.71	Joback Method
cpg	1002.82	J/mol×K	998.22	Joback Method

cpg	1018.12	J/mol×K	1043.73	Joback Method
cpg	1030.72	J/mol×K	1089.25	Joback Method
cpg	1040.72	J/mol×K	1134.76	Joback Method
dvisc	0.0007406	Pa×s	428.62	Joback Method
dvisc	0.0001812	Pa×s	500.80	Joback Method
dvisc	0.0000632	Pa×s	572.97	Joback Method
dvisc	0.0000279	Pa×s	645.15	Joback Method
dvisc	0.0000145	Pa×s	717.33	Joback Method
dvisc	0.0000085	Pa×s	789.50	Joback Method
dvisc	0.0000055	Pa×s	861.68	Joback Method
hsubt	108.80 ± 0.80	kJ/mol	361.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4384230&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
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