2,2-Metaparacyclophane

Inchi: InChI=1S/C16H16/c1-2-15-10-8-13-4-6-14(7-5-13)9-11-16(3-1)12-15/h1-7,12H,8-11H2
InchiKey: ALDQBAILWKRGEG-UHFFFAOYSA-N
Formula: C16H16
SMILES: c1cc2cc(c1)CCc1ccc(cc1)CC2
Mol. weight [g/mol]: 208.30
CAS: 5385-36-4

Physical Properties

Property code	Value	Unit	Source
chs	-8713.70 ± 1.30	kJ/mol	NIST Webbook
gf	345.76	kJ/mol	Joback Method
hf	218.30 ± 3.10	kJ/mol	NIST Webbook
hfs	130.80 ± 2.10	kJ/mol	NIST Webbook
hfus	19.46	kJ/mol	Joback Method
hsub	87.50 ± 0.90	kJ/mol	NIST Webbook
hsub	87.50	kJ/mol	NIST Webbook
hsub	88.00 ± 2.00	kJ/mol	NIST Webbook
hvap	57.48	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	3.570		Crippen Method
mcvol	177.920	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
tb	644.48	K	Joback Method
tc	901.88	K	Joback Method
tf	366.62	K	Joback Method
vc	0.665	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.42	J/mol×K	858.98	Joback Method
cpg	551.01	J/mol×K	901.88	Joback Method
cpg	456.99	J/mol×K	644.48	Joback Method
cpg	476.19	J/mol×K	687.38	Joback Method

cpg	493.79	J/mol×K	730.28	Joback Method
cpg	509.95	J/mol×K	773.18	Joback Method
cpg	524.78	J/mol×K	816.08	Joback Method
dvisc	0.0002378	Pa×s	644.48	Joback Method
dvisc	0.0002926	Pa×s	598.17	Joback Method
dvisc	0.0018114	Pa×s	366.62	Joback Method
dvisc	0.0010682	Pa×s	412.93	Joback Method
dvisc	0.0007007	Pa×s	459.24	Joback Method
dvisc	0.0004965	Pa×s	505.55	Joback Method
dvisc	0.0003728	Pa×s	551.86	Joback Method
hfust	12.76	kJ/mol	354.00	NIST Webbook
hsubt	86.60	kJ/mol	319.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5385364&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
hfust: Enthalpy of fusion at a given temperature
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