[2.2]Paracyclophane

Other names:	Cyclobis(benzene-1,4-dimethylene)
	Di-1,4-xylylene
	Di-p-xylylene
	Tricyclo[8.2.2.2(4,7)]hexadeca-4,6,10,12,13,15-hexaene
	tricyclo[8.2.2.24,7]hexadeca-1(12),4,6,10,13,15-hexaene
Inchi:	InChI=1S/C16H16/c1-2-14-4-3-13(1)9-10-15-5-7-16(8-6-15)12-11-14/h1-8H,9-12H2
InchiKey:	OOLUVSIJOMLOCB-UHFFFAOYSA-N
Formula:	C16H16
SMILES:	c1cc2ccc1CCc1ccc(cc1)CC2
Mol. weight [g/mol]:	208.30
CAS:	1633-22-3

Physical Properties

Property code	Value	Unit	Source
chs	-8727.57 ± 0.63	kJ/mol	NIST Webbook
chs	-8729.50 ± 1.80	kJ/mol	NIST Webbook
chs	-8737.00 ± 4.00	kJ/mol	NIST Webbook
gf	345.76	kJ/mol	Joback Method
hf	244.70 ± 2.10	kJ/mol	NIST Webbook
hf	241.30 ± 4.30	kJ/mol	NIST Webbook
hf	241.00 ± 4.20	kJ/mol	NIST Webbook
hfs	154.00 ± 4.00	kJ/mol	NIST Webbook
hfs	144.70 ± 0.88	kJ/mol	NIST Webbook
hfs	146.70 ± 2.80	kJ/mol	NIST Webbook
hfus	19.46	kJ/mol	Joback Method
hsub	96.20 ± 4.20	kJ/mol	NIST Webbook
hsub	96.30	kJ/mol	NIST Webbook
hsub	96.20 ± 4.20	kJ/mol	NIST Webbook
hsub	98.00	kJ/mol	NIST Webbook
hsub	87.30	kJ/mol	NIST Webbook
hvap	57.48	kJ/mol	Joback Method
ie	7.60	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.10	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
ie	8.08	eV	NIST Webbook

ie	7.80	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
ie	7.80	eV	NIST Webbook
log10ws	-4.55		Crippen Method
logp	3.570		Crippen Method
mcvol	177.920	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
ss	265.68	J/mol×K	NIST Webbook
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	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
cpg	538.42	J/mol×K	858.98	Joback Method
cpg	551.01	J/mol×K	901.88	Joback Method
cps	252.70	J/mol×K	298.15	NIST Webbook
cps	252.34	J/mol×K	298.15	NIST Webbook
cps	248.10	J/mol×K	300.00	NIST Webbook
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
dvisc	0.0002926	Pa×s	598.17	Joback Method
dvisc	0.0002378	Pa×s	644.48	Joback Method
hfust	0.21	kJ/mol	323.20	NIST Webbook
hsubt	99.60 ± 1.80	kJ/mol	381.40	NIST Webbook
hsubt	96.40 ± 1.50	kJ/mol	381.00	NIST Webbook
hsubt	92.90 ± 0.84	kJ/mol	363.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	3.02554e+01
Coeff. B	-1.42454e+04
Temperature range (K), min.	475.36
Temperature range (K), max.	571.10

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1633223&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume