(2.2)Metacyclophane

Other names:	Tricyclo[9.3.1.1^{4,8}]hexadeca-1(15),4,6,8(16),11,13-hexaene
	Di-m-xylylene
	Di-1,3-xylylene
	Tricyclo(9.3.1.14,8)hexadeca-1(15),4,6,8(16),11,13-hexaene
	Triple-layered-(2.2)metacyclophane
Inchi:	InChI=1S/C16H16/c1-3-13-7-9-15-5-2-6-16(12-15)10-8-14(4-1)11-13/h1-6,11-12H,7-10H
InchiKey:	COTONUHLIMVDNV-UHFFFAOYSA-N
Formula:	C16H16
SMILES:	c1cc2cc(c1)CCc1cccc(c1)CC2
Mol. weight [g/mol]:	208.30
CAS:	2319-97-3

Physical Properties

Property code	Value	Unit	Source
chs	-8661.30 ± 6.30	kJ/mol	NIST Webbook
gf	345.76	kJ/mol	Joback Method
hf	170.00 ± 7.90	kJ/mol	NIST Webbook
hfs	78.20 ± 6.30	kJ/mol	NIST Webbook
hfus	19.46	kJ/mol	Joback Method
hsub	91.80	kJ/mol	NIST Webbook
hsub	92.00 ± 2.00	kJ/mol	NIST Webbook
hsub	92.00 ± 2.00	kJ/mol	NIST Webbook
hvap	57.48	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
ie	8.24	eV	NIST Webbook
ie	8.24	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
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	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	551.01	J/mol×K	901.88	Joback Method
cps	240.60	J/mol×K	300.00	NIST Webbook
dvisc	0.0002378	Pa×s	644.48	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
dvisc	0.0002926	Pa×s	598.17	Joback Method
hfust	21.42	kJ/mol	404.00	NIST Webbook
hsubt	91.60 ± 1.70	kJ/mol	320.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2319973&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume