

Tricyclo[10.2.2.2(5,8)]octadeca-5,7,12,14,15,17-hex

Other names:	[3.3]Paracyclophane [3,3']-Paracyclophane Tricyclo[10.2.2.25,8]octadeca-5,7,12,14,15,17-hexaene
Inchi:	InChI=1S/C18H20/c1-3-15-7-11-17(12-8-15)5-2-6-18-13-9-16(4-1)10-14-18/h7-14H,1-6H
InchiKey:	RUVOYPXKKKFOGBH-UHFFFAOYSA-N
Formula:	C18H20
SMILES:	c1cc2ccc1CCc1ccc(cc1)CCC2
Mol. weight [g/mol]:	236.35
CAS:	2913-24-8

Physical Properties

Property code	Value	Unit	Source
chs	-9967.80 ± 1.80	kJ/mol	NIST Webbook
gf	338.40	kJ/mol	Joback Method
hf	129.40 ± 3.70	kJ/mol	NIST Webbook
hfs	26.20 ± 2.60	kJ/mol	NIST Webbook
hfus	20.44	kJ/mol	Joback Method
hsub	103.20	kJ/mol	NIST Webbook
hsub	103.30 ± 1.00	kJ/mol	NIST Webbook
hvap	62.28	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.351		Crippen Method
mcvol	206.100	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
tb	698.78	K	Joback Method
tc	961.20	K	Joback Method
tf	382.12	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.26	J/mol×K	961.20	Joback Method
cpg	658.71	J/mol×K	917.46	Joback Method

cpg	643.81	J/mol×K	873.73	Joback Method
cpg	627.43	J/mol×K	829.99	Joback Method
cpg	609.45	J/mol×K	786.25	Joback Method
cpg	589.75	J/mol×K	742.52	Joback Method
cpg	568.21	J/mol×K	698.78	Joback Method
cps	324.30	J/mol×K	300.00	NIST Webbook
dvisc	0.0004569	Pa×s	487.67	Joback Method
dvisc	0.0001071	Pa×s	698.78	Joback Method
dvisc	0.0017212	Pa×s	382.12	Joback Method
dvisc	0.0001408	Pa×s	646.00	Joback Method
dvisc	0.0001944	Pa×s	593.23	Joback Method
dvisc	0.0002859	Pa×s	540.45	Joback Method
dvisc	0.0008182	Pa×s	434.90	Joback Method
hfust	11.76	kJ/mol	377.00	NIST Webbook
hsubt	103.00 ± 1.00	kJ/mol	332.50	NIST Webbook
hsubt	97.80	kJ/mol	332.00	NIST Webbook

Sources

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=C2913248&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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