Tricyclo[8.2.2.2^{4,7}]hexadeca-6,10,12,5,6,11,12,13,15-hexamethyl-

Other names: 2,2,5,5',5,6'-Hexamethyl-[2.2]paracyclophane
Tricyclo[8.2.2.2

Inchi: InChI=1S/C22H28/c1-13-14(2)20-8-7-19(13)9-11-21-15(3)17(5)22(12-10-20)18(6)16(21)4

InchiKey: COWSCXIHIVAWAL-UHFFFAOYSA-N

Formula: C22H28

SMILES: Cc1c2ccc(c1C)CCc1c(C)c(C)c(c(C)c1C)CC2

Mol. weight [g/mol]: 292.46

CAS: 77897-17-7

Physical Properties

Property code	Value	Unit	Source
gf	338.50	kJ/mol	Joback Method
hf	-29.13	kJ/mol	Joback Method
hfus	32.67	kJ/mol	Joback Method
hvap	74.81	kJ/mol	Joback Method
ie	7.00	eV	NIST Webbook
ie	7.45 ± 0.05	eV	NIST Webbook
log10ws	-7.41		Crippen Method
logp	5.421		Crippen Method
mcvol	262.460	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
tb	811.64	K	Joback Method
tc	1044.04	K	Joback Method
tf	509.36	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.88	J/mol×K	811.64	Joback Method
cpg	804.22	J/mol×K	850.37	Joback Method
cpg	822.32	J/mol×K	889.11	Joback Method
cpg	839.23	J/mol×K	927.84	Joback Method
cpg	855.02	J/mol×K	966.57	Joback Method

cpg	869.77	J/mol×K	1005.31	Joback Method
cpg	883.54	J/mol×K	1044.04	Joback Method
dvisc	0.0005999	Pa×s	509.36	Joback Method
dvisc	0.0004225	Pa×s	559.74	Joback Method
dvisc	0.0003153	Pa×s	610.12	Joback Method
dvisc	0.0002461	Pa×s	660.50	Joback Method
dvisc	0.0001989	Pa×s	710.88	Joback Method
dvisc	0.0001653	Pa×s	761.26	Joback Method
dvisc	0.0001406	Pa×s	811.64	Joback Method

Sources

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=C77897177&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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