Tricyclo[8.2.2.2^{4,4}]hexadeca-5,6,10,11,12,13,14,15-octamethyl-

Other names: 2,2,5,6,2',3',5',6'-Octamethyl[2.2]paracyclophane
1,4,5,8,12,13,16,17-Octamethyltricyclo[8.2.2.2

Inchi: InChI=1S/C24H32/c1-13-14(2)22-11-12-24-19(7)17(5)23(18(6)20(24)8)10-9-21(13)15(3)

InchiKey: RLLDLOKLZDZVGV-UHFFFAOYSA-N

Formula: C24H32

SMILES: Cc1c(C)c2c(C)c(C)c1CCc1c(C)c(C)c(c(C)c1C)CC2

Mol. weight [g/mol]: 320.51

CAS: 77897-20-2

Physical Properties

Property code	Value	Unit	Source
gf	336.08	kJ/mol	Joback Method
hf	-93.35	kJ/mol	Joback Method
hfus	37.07	kJ/mol	Joback Method
hvap	80.58	kJ/mol	Joback Method
ie	7.15 ± 0.05	eV	NIST Webbook
ie	6.90	eV	NIST Webbook
log10ws	-8.36		Crippen Method
logp	6.038		Crippen Method
mcvol	290.640	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
tb	867.36	K	Joback Method
tc	1095.41	K	Joback Method
tf	556.94	K	Joback Method
vc	1.113	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	902.76	J/mol×K	867.36	Joback Method
cpg	922.08	J/mol×K	905.37	Joback Method
cpg	940.16	J/mol×K	943.38	Joback Method
cpg	957.05	J/mol×K	981.39	Joback Method
cpg	972.82	J/mol×K	1019.40	Joback Method

cpg	987.51	J/mol×K	1057.40	Joback Method
cpg	1001.19	J/mol×K	1095.41	Joback Method
dvisc	0.0004457	Pa×s	556.94	Joback Method
dvisc	0.0003250	Pa×s	608.68	Joback Method
dvisc	0.0002490	Pa×s	660.41	Joback Method
dvisc	0.0001983	Pa×s	712.15	Joback Method
dvisc	0.0001629	Pa×s	763.89	Joback Method
dvisc	0.0001371	Pa×s	815.62	Joback Method
dvisc	0.0001179	Pa×s	867.36	Joback Method

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=C77897202&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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