Tricyclo[8.2.2.2^{4,7}]octadeca-4,6,10,1

Other names: [2.2]1,6-Cyclooctatetraenyl-1,4-cyclophane
Tricyclo[8.2.2.2
Inchi: InChI=1S/C18H18/c1-2-4-16-6-5-15(3-1)7-9-17-11-13-18(10-8-16)14-12-17/h1-6,11-14H
InchiKey: VRGLNGRQXLSACG-IGWMJARQSA-N
Formula: C18H18
SMILES: C1=CC=C2C=CC(=C1)CCc1ccc(cc1)CC2
Mol. weight [g/mol]: 234.34
CAS: 84954-88-1

Physical Properties

Property code	Value	Unit	Source
gf	368.36	kJ/mol	Joback Method
hf	167.71	kJ/mol	Joback Method
hfus	21.67	kJ/mol	Joback Method
hvap	62.57	kJ/mol	Joback Method
ie	7.65	eV	NIST Webbook
ie	7.30	eV	NIST Webbook
log10ws	-5.63		Crippen Method
logp	4.544		Crippen Method
mcvol	201.800	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	697.94	K	Joback Method
tc	962.92	K	Joback Method
tf	382.88	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.10	J/mol×K	697.94	Joback Method
cpg	564.50	J/mol×K	742.10	Joback Method
cpg	583.11	J/mol×K	786.27	Joback Method
cpg	600.05	J/mol×K	830.43	Joback Method
cpg	615.46	J/mol×K	874.59	Joback Method

cpg	629.46	J/mol×K	918.76	Joback Method
cpg	642.17	J/mol×K	962.92	Joback Method
dvisc	0.0015907	Pa×s	382.88	Joback Method
dvisc	0.0007841	Pa×s	435.39	Joback Method
dvisc	0.0004501	Pa×s	487.90	Joback Method
dvisc	0.0002878	Pa×s	540.41	Joback Method
dvisc	0.0001991	Pa×s	592.92	Joback Method
dvisc	0.0001463	Pa×s	645.43	Joback Method
dvisc	0.0001126	Pa×s	697.94	Joback Method

Sources

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=C84954881&Units=SI

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