

Anti-7,14-dihydro-7,14-bis(2-propylidene)-1,6:8,13

Inchi:	InChI=1S/C22H24/c1-15(2)21-17-9-5-7-11-19(13-17)22(16(3)4)20-12-8-6-10-18(21)14-2
InchiKey:	SDQUZEYARJZOCM-UHFFFAOYSA-N
Formula:	C22H24
SMILES:	CC(C)=C1C2=CC=CC=C(C2)C(=C(C)C)C2=CC=CC=C1C2
Mol. weight [g/mol]:	288.43
CAS:	109281-34-7

Physical Properties

Property code	Value	Unit	Source
gf	470.10	kJ/mol	Joback Method
hf	172.17	kJ/mol	Joback Method
hfus	33.03	kJ/mol	Joback Method
hvap	72.57	kJ/mol	Joback Method
ie	6.90	eV	NIST Webbook
ie	7.00	eV	NIST Webbook
log10ws	-7.55		Crippen Method
logp	6.298		Crippen Method
mcvol	253.860	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
tb	794.80	K	Joback Method
tc	1041.26	K	Joback Method
tf	427.04	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.95	J/molxK	794.80	Joback Method
cpg	752.97	J/molxK	835.88	Joback Method
cpg	770.70	J/molxK	876.95	Joback Method
cpg	787.28	J/molxK	918.03	Joback Method
cpg	802.87	J/molxK	959.11	Joback Method
cpg	817.61	J/molxK	1000.18	Joback Method
cpg	831.66	J/molxK	1041.26	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=C109281347&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
h vap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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