

Hexacyclo[7:2:1:0(2,5):0(3,10):0(4,8):0(6,12)]dodac

Inchi: InChI=1S/C12H14/c1-3-7-5-2-6-8(7)4(1)10-9(3)11(5)12(6)10/h3-12H,1-2H2
InchiKey: VTRWGAFQJZEOAR-UHFFFAOYSA-N
Formula: C12H14
SMILES: C1C2C3C4CC5C3C1C1C2C4C51
Mol. weight [g/mol]: 158.24
CAS: 704-02-9

Physical Properties

Property code	Value	Unit	Source
chs	-6773.48	kJ/mol	NIST Webbook
gf	456.42	kJ/mol	Joback Method
hf	101.39	kJ/mol	Joback Method
hfs	50.50 ± 1.10	kJ/mol	NIST Webbook
hfus	32.53	kJ/mol	Joback Method
hvap	39.52	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	2.010		Crippen Method
mcvol	114.780	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
tb	470.10	K	Joback Method
tc	670.74	K	Joback Method
tf	336.80	K	Joback Method
vc	0.493	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.54	J/mol×K	470.10	Joback Method
cpg	410.49	J/mol×K	637.30	Joback Method
cpg	396.20	J/mol×K	603.86	Joback Method
cpg	380.64	J/mol×K	570.42	Joback Method
cpg	363.63	J/mol×K	536.98	Joback Method
cpg	344.99	J/mol×K	503.54	Joback Method
cpg	423.69	J/mol×K	670.74	Joback Method

dvisc	0.0280279	Paxs	470.10	Joback Method
dvisc	0.0185223	Paxs	447.88	Joback Method
dvisc	0.0117225	Paxs	425.67	Joback Method
dvisc	0.0070545	Paxs	403.45	Joback Method
dvisc	0.0040013	Paxs	381.23	Joback Method
dvisc	0.0021158	Paxs	359.02	Joback Method
dvisc	0.0010285	Paxs	336.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C704029&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas 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
hvap:	Enthalpy of vaporization at standard conditions
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

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