

Pentacyclo[6.3.1.0(2,7).0(3,5).0(9,11)]dodecane

Inchi:	InChI=1S/C12H16/c1-5-2-10-9-4-11(8-3-7(8)9)12(10)6(1)5/h5-12H,1-4H2
InchiKey:	CUEVXBHHOPVSBW-UHFFFAOYSA-N
Formula:	C12H16
SMILES:	C1C2C3CC(C12)C1C2CC2CC31
Mol. weight [g/mol]:	160.26
CAS:	82110-70-1

Physical Properties

Property code	Value	Unit	Source
chl	-7136.30 ± 3.90	kJ/mol	NIST Webbook
gf	367.08	kJ/mol	Joback Method
hf	185.50	kJ/mol	NIST Webbook
hfl	127.50 ± 3.90	kJ/mol	NIST Webbook
hfus	27.02	kJ/mol	Joback Method
hvap	58.00	kJ/mol	NIST Webbook
hvap	58.00	kJ/mol	NIST Webbook
log10ws	-2.39		Crippen Method
logp	2.544		Crippen Method
mcvol	125.640	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
tb	480.84	K	Joback Method
tc	689.03	K	Joback Method
tf	312.54	K	Joback Method
vc	0.513	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.00	J/mol×K	480.84	Joback Method
cpg	360.60	J/mol×K	515.54	Joback Method
cpg	380.45	J/mol×K	550.24	Joback Method
cpg	398.72	J/mol×K	584.94	Joback Method
cpg	415.57	J/mol×K	619.63	Joback Method
cpg	431.15	J/mol×K	654.33	Joback Method

cpg	445.62	J/molxK	689.03	Joback Method
dvisc	0.0006245	Paxs	312.54	Joback Method
dvisc	0.0012137	Paxs	340.59	Joback Method
dvisc	0.0021322	Paxs	368.64	Joback Method
dvisc	0.0034587	Paxs	396.69	Joback Method
dvisc	0.0052633	Paxs	424.74	Joback Method
dvisc	0.0076034	Paxs	452.79	Joback Method
dvisc	0.0105226	Paxs	480.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82110701&Units=SI
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

Legend

chl:	Standard liquid 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
hfl:	Liquid 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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