

Helifolen-12-al-D, syn-syn-syn

Inchi:	InChI=1S/C15H20O/c1-10-3-4-12-13(2,9-16)11-5-6-14(11)7-8-15(10,12)14/h5-6,9-12H,3
InchiKey:	XYBQLTCBTATXFX-UHFFFAOYSA-N
Formula:	C15H20O
SMILES:	CC1CCC2C(C)(C=O)C3C=CC34CCC124
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
gf	216.97	kJ/mol	Joback Method
hf	-84.49	kJ/mol	Joback Method
hfus	13.90	kJ/mol	Joback Method
hvap	51.58	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.204		Crippen Method
mcvol	176.040	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinqol	1621.00		NIST Webbook
tb	608.76	K	Joback Method
tc	845.25	K	Joback Method
tf	436.55	K	Joback Method
vc	0.699	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.89	J/mol×K	608.76	Joback Method
cpg	530.24	J/mol×K	648.18	Joback Method
cpg	548.31	J/mol×K	687.59	Joback Method
cpg	565.63	J/mol×K	727.01	Joback Method
cpg	582.71	J/mol×K	766.42	Joback Method
cpg	600.06	J/mol×K	805.84	Joback Method
cpg	618.20	J/mol×K	845.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R587385&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

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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