helifolen-12-al (anti-syn-syn)

Inchi: InChI=1S/C15H22O/c1-11-4-5-12-14(3,10-16)13(2)6-8-15(11,12)9-7-13/h6,8,10-12H,4-5
InchiKey: IVGPPCYQIKEJMO-UHFFFAOYSA-N
Formula: C15H22O
SMILES: CC1CCC2C13C=CC(C)(CC3)C2(C)C=O
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	132.02	kJ/mol	Joback Method
hf	-169.61	kJ/mol	Joback Method
hfus	11.57	kJ/mol	Joback Method
hvap	52.01	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2405.28	kPa	Joback Method
rinpol	1606.00		NIST Webbook
rinpol	1606.00		NIST Webbook
tb	610.56	K	Joback Method
tc	846.37	K	Joback Method
tf	411.57	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	528.43	J/mol×K	610.56	Joback Method
cpg	549.02	J/mol×K	649.86	Joback Method
cpg	568.38	J/mol×K	689.16	Joback Method
cpg	586.96	J/mol×K	728.46	Joback Method
cpg	605.21	J/mol×K	767.77	Joback Method
cpg	623.58	J/mol×K	807.07	Joback Method
cpg	642.54	J/mol×K	846.37	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=R233642&Units=SI

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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