7-epi-Helifolan-12-ol (syn)

Inchi: InChI=1S/C15H24O/c1-11-4-5-12-14(3,10-16)13(2)6-8-15(11,12)9-7-13/h6,8,11-12,16H,4
InchiKey: AGJMNKNZLOUBMN-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1CCC2C13C=CC(C)(CC3)C2(C)CO
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	94.72	kJ/mol	Joback Method
hf	-236.26	kJ/mol	Joback Method
hfus	13.37	kJ/mol	Joback Method
hvap	61.97	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.387		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1697.00		NIST Webbook
rinpol	1697.00		NIST Webbook
ripol	2446.00		NIST Webbook
tb	654.08	K	Joback Method
tc	869.33	K	Joback Method
tf	430.39	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.29	J/mol×K	654.08	Joback Method
cpg	589.81	J/mol×K	689.96	Joback Method
cpg	607.66	J/mol×K	725.83	Joback Method
cpg	625.17	J/mol×K	761.71	Joback Method
cpg	642.71	J/mol×K	797.58	Joback Method
cpg	660.61	J/mol×K	833.46	Joback Method
cpg	679.23	J/mol×K	869.33	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=R503030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume