Helifolen-12-oic acid (anti-anti-anti), methyl ester

Inchi: InChI=1S/C16H24O2/c1-11-5-6-12-15(3,13(17)18-4)14(2)7-9-16(11,12)10-8-14/h7,9,11-1

InchiKey: BGRIBZWMDPIJFU-UHFFFAOYSA-N

Formula: C16H24O2

SMILES: COC(=O)C1(C)C2CCC(C)C23C=CC1(C)CC3

Mol. weight [g/mol]: 248.36

Physical Properties

Property code	Value	Unit	Source
gf	6.04	kJ/mol	Joback Method
hf	-349.47	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	56.67	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.568		Crippen Method
mcvol	206.860	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	1655.00		NIST Webbook
ripol	2050.00		NIST Webbook
ripol	2050.00		NIST Webbook
tb	661.07	K	Joback Method
tc	893.85	K	Joback Method
tf	453.00	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.03	J/mol×K	661.07	Joback Method
cpg	630.94	J/mol×K	699.87	Joback Method
cpg	651.10	J/mol×K	738.66	Joback Method
cpg	670.92	J/mol×K	777.46	Joback Method
cpg	690.83	J/mol×K	816.26	Joback Method
cpg	711.25	J/mol×K	855.05	Joback Method
cpg	732.59	J/mol×K	893.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R503070&Units=SI
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

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