Methyl syn-3-Hydroxymethyl-helifolen-12-oate

Inchi: InChI=1S/C16H24O3/c1-11-4-5-12-14(2,13(18)19-3)15(10-17)6-8-16(11,12)9-7-15/h6,8,1
InchiKey: JYLSKFICMHIFPA-UHFFFAOYSA-N
Formula: C16H24O3
SMILES: COC(=O)C1(C)C2CCC(C)C23C=CC1(CO)CC3
Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
gf	-130.78	kJ/mol	Joback Method
hf	-501.70	kJ/mol	Joback Method
hfus	18.75	kJ/mol	Joback Method
hvap	73.35	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.540		Crippen Method
mcvol	212.730	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	1905.00		NIST Webbook
rinpol	1905.00		NIST Webbook
tb	753.25	K	Joback Method
tc	969.18	K	Joback Method
tf	513.82	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.39	J/mol×K	753.25	Joback Method
cpg	694.93	J/mol×K	789.24	Joback Method
cpg	713.63	J/mol×K	825.23	Joback Method
cpg	732.83	J/mol×K	861.21	Joback Method
cpg	752.87	J/mol×K	897.20	Joback Method
cpg	774.09	J/mol×K	933.19	Joback Method
cpg	796.82	J/mol×K	969.18	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=R503352&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume