Methyl syn-3-Formyl-helifolen-12-oate

Inchi: InChI=1S/C16H22O3/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: RCPDICCZCVVSPJ-UHFFFAOYSA-N
Formula: C16H22O3
SMILES: COC(=O)C1(C)C2CCC(C)C23C=CC1(C=O)CC3
Mol. weight [g/mol]: 262.34

Physical Properties

Property code	Value	Unit	Source
gf	-93.48	kJ/mol	Joback Method
hf	-435.05	kJ/mol	Joback Method
hfus	16.95	kJ/mol	Joback Method
hvap	63.39	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	2.747		Crippen Method
mcvol	208.430	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1793.00		NIST Webbook
rinpol	1793.00		NIST Webbook
tb	709.73	K	Joback Method
tc	943.49	K	Joback Method
tf	495.00	K	Joback Method
vc	0.805	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.18	J/mol×K	709.73	Joback Method
cpg	651.57	J/mol×K	748.69	Joback Method
cpg	670.74	J/mol×K	787.65	Joback Method
cpg	690.11	J/mol×K	826.61	Joback Method
cpg	710.12	J/mol×K	865.57	Joback Method
cpg	731.17	J/mol×K	904.53	Joback Method
cpg	753.70	J/mol×K	943.49	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=R503347&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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