Ilicic acid, methyl ester

Inchi: InChI=1S/C16H26O3/c1-11(14(17)19-4)12-6-9-15(2)7-5-8-16(3,18)13(15)10-12/h12-13,1
InchiKey: PMRPCJXLEQCTBH-BGHVQYPCSA-N
Formula: C16H26O3
SMILES: C=C(C(=O)OC)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]: 266.38

Physical Properties

Property code	Value	Unit	Source
gf	-160.91	kJ/mol	Joback Method
hf	-544.20	kJ/mol	Joback Method
hfus	18.90	kJ/mol	Joback Method
hvap	74.05	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.073		Crippen Method
mcvol	223.590	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1966.00		NIST Webbook
tb	752.21	K	Joback Method
tc	966.12	K	Joback Method
tf	448.46	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.70	J/mol×K	752.21	Joback Method
cpg	723.18	J/mol×K	787.86	Joback Method
cpg	742.20	J/mol×K	823.51	Joback Method
cpg	760.98	J/mol×K	859.17	Joback Method
cpg	779.71	J/mol×K	894.82	Joback Method
cpg	798.62	J/mol×K	930.47	Joback Method
cpg	817.90	J/mol×K	966.12	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=R510786&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