«beta»-cyclogeraniumacid methyl ester

Inchi: InChI=1S/C11H18O2/c1-11(2)6-4-5-9(8-11)7-10(12)13-3/h8H,4-7H2,1-3H3
InchiKey: SZONIZYCGSWBFY-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: COC(=O)CC1=CC(C)(C)CCC1
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-152.89	kJ/mol	Joback Method
hf	-399.30	kJ/mol	Joback Method
hfus	13.40	kJ/mol	Joback Method
hvap	49.47	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.686		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
rinpol	1235.00		NIST Webbook
tb	551.30	K	Joback Method
tc	764.81	K	Joback Method
tf	330.45	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.71	J/mol×K	551.30	Joback Method
cpg	401.63	J/mol×K	586.89	Joback Method
cpg	417.59	J/mol×K	622.47	Joback Method
cpg	432.70	J/mol×K	658.06	Joback Method
cpg	447.04	J/mol×K	693.64	Joback Method
cpg	460.71	J/mol×K	729.23	Joback Method
cpg	473.80	J/mol×K	764.81	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=R226149&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