Methyl-«gamma»-Cyclogeranate

Inchi: InChI=1S/C11H18O2/c1-8-6-5-7-11(2,3)9(8)10(12)13-4/h9H,1,5-7H2,2-4H3
InchiKey: SMJXJPQSPQXVMU-UHFFFAOYSA-N
Formula: C11H18O2
SMILES: C=C1CCCC(C)(C)C1C(=O)OC
Mol. weight [g/mol]: 182.26

Physical Properties

Property code	Value	Unit	Source
gf	-127.85	kJ/mol	Joback Method
hf	-381.71	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	48.36	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.542		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2520.12	kPa	Joback Method
rinpol	1184.00		NIST Webbook
tb	541.65	K	Joback Method
tc	753.77	K	Joback Method
tf	326.61	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.81	J/mol×K	541.65	Joback Method
cpg	402.36	J/mol×K	577.00	Joback Method
cpg	418.95	J/mol×K	612.36	Joback Method
cpg	434.68	J/mol×K	647.71	Joback Method
cpg	449.61	J/mol×K	683.06	Joback Method
cpg	463.84	J/mol×K	718.42	Joback Method
cpg	477.44	J/mol×K	753.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R229282&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume