1-Cyclohexene-1-carboxylic acid, 2,6,6-trimethyl-, methyl ester

Other names: Methyl-«beta»-Cyclogeranate
cgm

Inchi: InChI=1S/C11H18O2/c1-8-6-5-7-11(2,3)9(8)10(12)13-4/h5-7H2,1-4H3

InchiKey: NNSDFWCDDSJPFI-UHFFFAOYSA-N

Formula: C11H18O2

SMILES: COC(=O)C1=C(C)CCCC1(C)C

Mol. weight [g/mol]: 182.26

CAS: 49815-58-9

Physical Properties

Property code	Value	Unit	Source
gf	-162.52	kJ/mol	Joback Method
hf	-410.77	kJ/mol	Joback Method
hfus	13.01	kJ/mol	Joback Method
hvap	50.13	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.686		Crippen Method
mcvol	158.130	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1224.00		NIST Webbook
rinpol	1224.00		NIST Webbook
ripol	1570.00		NIST Webbook
tb	556.28	K	Joback Method
tc	770.86	K	Joback Method
tf	342.97	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.81	J/mol×K	556.28	Joback Method
cpg	401.41	J/mol×K	592.04	Joback Method
cpg	417.13	J/mol×K	627.81	Joback Method
cpg	432.04	J/mol×K	663.57	Joback Method

cpg	446.24	J/mol×K	699.33	Joback Method
cpg	459.81	J/mol×K	735.10	Joback Method
cpg	472.85	J/mol×K	770.86	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=C49815589&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume