1-carbomethoxy-1-methylcyclohex-3-ene

Inchi: InChI=1S/C9H14O2/c1-9(8(10)11-2)6-4-3-5-7-9/h3-4H,5-7H2,1-2H3
InchiKey: GLCJULYDLTXOEN-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: COC(=O)C1(C)CC=CCC1
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
gf	-160.10	kJ/mol	Joback Method
hf	-346.55	kJ/mol	Joback Method
hfus	8.61	kJ/mol	Joback Method
hvap	44.35	kJ/mol	Joback Method
log10ws	-1.96		Crippen Method
logp	1.906		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
ripol	1442.00		NIST Webbook
ripol	1458.40		NIST Webbook
ripol	1442.00		NIST Webbook
tb	500.56	K	Joback Method
tc	720.15	K	Joback Method
tf	295.39	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.56	J/mol×K	500.56	Joback Method
cpg	307.34	J/mol×K	537.16	Joback Method
cpg	322.09	J/mol×K	573.76	Joback Method
cpg	335.92	J/mol×K	610.36	Joback Method
cpg	348.93	J/mol×K	646.95	Joback Method
cpg	361.21	J/mol×K	683.55	Joback Method
cpg	372.87	J/mol×K	720.15	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R388277&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume