cis-1-carbomethoxy-5-tert-butylcyclohex-3-ene

Inchi: InChI=1S/C12H20O2/c1-12(2,3)10-7-5-6-9(8-10)11(13)14-4/h5,7,9-10H,6,8H2,1-4H3/t9-,
InchiKey: MWUJYSQXIKGVTI-VHSXEESVSA-N
Formula: C12H20O2
SMILES: COC(=O)C1CC=CC(C(C)(C)C)C1
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-134.22	kJ/mol	Joback Method
hf	-452.80	kJ/mol	Joback Method
hfus	16.34	kJ/mol	Joback Method
hvap	50.58	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.788		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
ripol	1728.50		NIST Webbook
ripol	1740.80		NIST Webbook
ripol	1728.50		NIST Webbook
tb	561.06	K	Joback Method
tc	774.40	K	Joback Method
tf	303.48	K	Joback Method
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.71	J/mol×K	561.06	Joback Method
cpg	458.34	J/mol×K	596.62	Joback Method
cpg	476.82	J/mol×K	632.17	Joback Method
cpg	494.16	J/mol×K	667.73	Joback Method
cpg	510.41	J/mol×K	703.28	Joback Method
cpg	525.59	J/mol×K	738.84	Joback Method
cpg	539.75	J/mol×K	774.40	Joback Method

dvisc	0.0033615	Pa×s	303.48	Joback Method
dvisc	0.0015922	Pa×s	346.41	Joback Method
dvisc	0.0008892	Pa×s	389.34	Joback Method
dvisc	0.0005576	Pa×s	432.27	Joback Method
dvisc	0.0003804	Pa×s	475.20	Joback Method
dvisc	0.0002765	Pa×s	518.13	Joback Method
dvisc	0.0002110	Pa×s	561.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R388391&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
dvisc:	Dynamic viscosity
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