

1-carbomethoxy-1-methyl-4-tert-butylcyclohex-3-ene

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C13H22O2/c1-12(2,3)10-6-8-13(4,9-7-10)11(14)15-5/h6H,7-9H2,1-5H3

RIFPBZLRCXOBTR-UHFFFAOYSA-N

C13H22O2

COC(=O)C1(C)CC=C(C(C)(C)C)CC1

210.31

Physical Properties

Property code	Value	Unit	Source
gf	-133.21	kJ/mol	Joback Method
hf	-449.33	kJ/mol	Joback Method
hfus	11.17	kJ/mol	Joback Method
hvap	52.62	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	3.322		Crippen Method
mcvol	186.310	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
ripol	1686.30		NIST Webbook
ripol	1686.30		NIST Webbook
tb	593.83	K	Joback Method
tc	812.92	K	Joback Method
tf	355.41	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.17	J/mol×K	593.83	Joback Method
cpg	506.28	J/mol×K	630.35	Joback Method
cpg	524.24	J/mol×K	666.86	Joback Method
cpg	541.18	J/mol×K	703.38	Joback Method
cpg	557.23	J/mol×K	739.89	Joback Method
cpg	572.52	J/mol×K	776.41	Joback Method
cpg	587.18	J/mol×K	812.92	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=R388257&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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