trans-carbomethoxy-1,2-methylcyclohex-3-ene

Inchi: InChI=1S/C10H16O2/c1-8-6-4-5-7-10(8,2)9(11)12-3/h4,6,8H,5,7H2,1-3H3/t8-,10-/m1/s1
InchiKey: NLOSWJVOKLFODS-PSASIEDQSA-N
Formula: C10H16O2
SMILES: COC(=O)C1(C)CCC=CC1C
Mol. weight [g/mol]: 168.23

Physical Properties

Property code	Value	Unit	Source
gf	-159.39	kJ/mol	Joback Method
hf	-387.53	kJ/mol	Joback Method
hfus	12.27	kJ/mol	Joback Method
hvap	46.27	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.152		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
ripol	1522.70		NIST Webbook
ripol	1549.20		NIST Webbook
ripol	1509.80		NIST Webbook
ripol	1509.80		NIST Webbook
tb	518.77	K	Joback Method
tc	734.61	K	Joback Method
tf	302.42	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.11	J/mol×K	518.77	Joback Method
cpg	355.11	J/mol×K	554.74	Joback Method
cpg	371.10	J/mol×K	590.72	Joback Method
cpg	386.17	J/mol×K	626.69	Joback Method
cpg	400.41	J/mol×K	662.66	Joback Method
cpg	413.92	J/mol×K	698.64	Joback Method

cpg	426.77	J/mol×K	734.61	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=R388415&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

Latest version available from:
https://www.chemeo.com/cid/94-500-2/trans-carbomethoxy-1-2-methylcyclohex-3-ene.pdf
Generated by Cheméo on 2024-02-27 10:01:40.383831659 +0000 UTC m=+11317349.304408975.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.