

trans-carbomethoxy-1,5-methylcyclohex-3-ene

Inchi:	InChI=1S/C10H16O2/c1-8-5-4-6-10(2,7-8)9(11)12-3/h4-5,8H,6-7H2,1-3H3/t8-,10-/m0/s1
InchiKey:	DPIKCQABJXNSJR-WPRPVWTQSA-N
Formula:	C10H16O2
SMILES:	COC(=O)C1(C)CC=CC(C)C1
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	1458.40		NIST Webbook
ripol	1426.30		NIST Webbook
ripol	1426.30		NIST Webbook
ripol	1437.50		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

Sources

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=R388440&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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