cis-1-carbomethoxy-5-methylcyclohex-3-ene

Inchi: InChI=1S/C9H14O2/c1-7-4-3-5-8(6-7)9(10)11-2/h3-4,7-8H,5-6H2,1-2H3/t7-,8+/m1/s1
InchiKey: VZAIBLBJANAOTQ-SFYZADRCSA-N
Formula: C9H14O2
SMILES: COC(=O)C1CC=CC(C)C1
Mol. weight [g/mol]: 154.21

Physical Properties

Property code	Value	Unit	Source
gf	-162.32	kJ/mol	Joback Method
hf	-382.13	kJ/mol	Joback Method
hfus	15.98	kJ/mol	Joback Method
hvap	45.20	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.762		Crippen Method
mcvol	129.950	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
ripol	1527.80		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1497.00		NIST Webbook
ripol	1530.40		NIST Webbook
tb	495.65	K	Joback Method
tc	705.97	K	Joback Method
tf	267.25	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.21	J/mol×K	495.65	Joback Method
cpg	308.44	J/mol×K	530.70	Joback Method
cpg	323.88	J/mol×K	565.76	Joback Method
cpg	338.53	J/mol×K	600.81	Joback Method
cpg	352.41	J/mol×K	635.86	Joback Method
cpg	365.52	J/mol×K	670.91	Joback Method

cpg	377.85	J/mol×K	705.97	Joback Method
dvisc	0.0026183	Pa×s	267.25	Joback Method
dvisc	0.0014230	Pa×s	305.32	Joback Method
dvisc	0.0008854	Pa×s	343.38	Joback Method
dvisc	0.0006056	Pa×s	381.45	Joback Method
dvisc	0.0004438	Pa×s	419.52	Joback Method
dvisc	0.0003424	Pa×s	457.58	Joback Method
dvisc	0.0002750	Pa×s	495.65	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=R388386&Units=SI

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

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