cis-Methylcyclopropanecarboxylate, 2-methyl-2-phenyl

Inchi: InChI=1S/C12H14O2/c1-12(8-10(12)11(13)14-2)9-6-4-3-5-7-9/h3-7,10H,8H2,1-2H3/t10-,

InchiKey: OTRGRBMQMYBGDZ-PWSUYJOCSA-N

Formula: C12H14O2

SMILES: COC(=O)C1CC1(C)c1ccccc1

Mol. weight [g/mol]: 190.24

Physical Properties

Property code	Value	Unit	Source
gf	-23.80	kJ/mol	Joback Method
hf	-231.58	kJ/mol	Joback Method
hfus	16.57	kJ/mol	Joback Method
hvap	52.19	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.137		Crippen Method
mcvol	152.760	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
rinpol	1300.00		NIST Webbook
tb	579.24	K	Joback Method
tc	809.21	K	Joback Method
tf	361.18	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.68	J/mol×K	579.24	Joback Method
cpg	395.68	J/mol×K	617.57	Joback Method
cpg	410.58	J/mol×K	655.90	Joback Method
cpg	424.55	J/mol×K	694.22	Joback Method
cpg	437.74	J/mol×K	732.55	Joback Method
cpg	450.31	J/mol×K	770.88	Joback Method
cpg	462.42	J/mol×K	809.21	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=R13549&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume