cis-Methyl 1,2-diphenylcyclopropane carboxylate

Inchi: InChI=1S/C17H16O2/c1-19-16(18)17(14-10-6-3-7-11-14)12-15(17)13-8-4-2-5-9-13/h2-11
InchiKey: YAOZVDIKXMRFBG-WBVHZDCISA-N
Formula: C17H16O2
SMILES: COC(=O)C1(c2ccccc2)CC1c1ccccc1
Mol. weight [g/mol]: 252.31
CAS: 36634-64-7

Physical Properties

Property code	Value	Unit	Source
gf	130.71	kJ/mol	Joback Method
hf	-98.25	kJ/mol	Joback Method
hfus	23.56	kJ/mol	Joback Method
hvap	65.60	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.285		Crippen Method
mcvol	199.450	ml/mol	McGowan Method
pc	2500.00	kPa	Joback Method
tb	720.32	K	Joback Method
tc	973.01	K	Joback Method
tf	443.95	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	554.91	J/mol×K	720.32	Joback Method
cpg	572.55	J/mol×K	762.44	Joback Method
cpg	589.19	J/mol×K	804.55	Joback Method
cpg	605.09	J/mol×K	846.67	Joback Method
cpg	620.48	J/mol×K	888.78	Joback Method
cpg	635.63	J/mol×K	930.90	Joback Method
cpg	650.76	J/mol×K	973.01	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=C36634647&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume