Methyl trans-2-phenyl-1-cyclopropanecarboxylate

Other names: Methyl 2-phenylcyclopropanecarboxylate, trans-
trans-Methylcyclopropanecarboxylate, 2-methyl-2-phenyl
Inchi: InChI=1S/C11H12O2/c1-13-11(12)10-7-9(10)8-5-3-2-4-6-8/h2-6,9-10H,7H2,1H3/t9-,10+/
InchiKey: BQRFZWGTJXCXSR-VHSXEESVSA-N
Formula: C11H12O2
SMILES: COC(=O)C1CC1c1ccccc1
Mol. weight [g/mol]: 176.21
CAS: 5861-31-4

Physical Properties

Property code	Value	Unit	Source
gf	-26.73	kJ/mol	Joback Method
hf	-226.18	kJ/mol	Joback Method
hfus	20.28	kJ/mol	Joback Method
hvap	51.12	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.963		Crippen Method
mcvol	138.670	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
rinpol	1375.00		NIST Webbook
tb	556.12	K	Joback Method
tc	781.18	K	Joback Method
tf	326.01	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.41	J/mol×K	556.12	Joback Method
cpg	349.06	J/mol×K	593.63	Joback Method
cpg	363.68	J/mol×K	631.14	Joback Method
cpg	377.31	J/mol×K	668.65	Joback Method
cpg	390.00	J/mol×K	706.16	Joback Method
cpg	401.79	J/mol×K	743.67	Joback Method

cpg	412.73	J/mol×K	781.18	Joback Method
dvisc	0.0017296	Pa×s	326.01	Joback Method
dvisc	0.0012587	Pa×s	364.36	Joback Method
dvisc	0.0009732	Pa×s	402.71	Joback Method
dvisc	0.0007868	Pa×s	441.06	Joback Method
dvisc	0.0006582	Pa×s	479.42	Joback Method
dvisc	0.0005653	Pa×s	517.77	Joback Method
dvisc	0.0004959	Pa×s	556.12	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=C5861314&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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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