Cyclopropane-1-carboxylic acid, 2-methoxymethyl-3-phenyl, ethyl ester

Inchi: InChI=1S/C14H18O3/c1-3-17-14(15)13-11(9-16-2)12(13)10-7-5-4-6-8-10/h4-8,11-13H,3,

InchiKey: XTXDOAAMPZLWCV-UHFFFAOYSA-N

Formula: C14H18O3

SMILES: CCOC(=O)C1C(COC)C1c1ccccc1

Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
gf	-114.18	kJ/mol	Joback Method
hf	-440.66	kJ/mol	Joback Method
hfus	30.31	kJ/mol	Joback Method
hvap	59.89	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.226		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1521.00		NIST Webbook
tb	642.51	K	Joback Method
tc	853.50	K	Joback Method
tf	377.81	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.90	J/mol×K	642.51	Joback Method
cpg	587.56	J/mol×K	818.33	Joback Method
cpg	574.21	J/mol×K	783.17	Joback Method
cpg	559.90	J/mol×K	748.00	Joback Method
cpg	544.60	J/mol×K	712.84	Joback Method
cpg	528.27	J/mol×K	677.67	Joback Method
cpg	599.96	J/mol×K	853.50	Joback Method
dvisc	0.0004213	Pa×s	642.51	Joback Method
dvisc	0.0004802	Pa×s	598.39	Joback Method

dvisc	0.0005590	Pa×s	554.28	Joback Method
dvisc	0.0006679	Pa×s	510.16	Joback Method
dvisc	0.0008254	Pa×s	466.04	Joback Method
dvisc	0.0010663	Pa×s	421.93	Joback Method
dvisc	0.0014623	Pa×s	377.81	Joback Method

Sources

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=R329496&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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