Cyclopropane-1-carboxylic acid, 2-methoxy-2-phenyl, ethyl ester, trans

Inchi: InChI=1S/C13H16O3/c1-3-16-12(14)11-9-13(11,15-2)10-7-5-4-6-8-10/h4-8,11H,3,9H2,1-

InchiKey: SMIKOOKFNIKEGW-DGCLKSJQSA-N

Formula: C13H16O3

SMILES: CCOC(=O)C1CC1(OC)c1ccccc1

Mol. weight [g/mol]: 220.26

Physical Properties

Property code	Value	Unit	Source
gf	-120.38	kJ/mol	Joback Method
hf	-384.44	kJ/mol	Joback Method
hfus	20.35	kJ/mol	Joback Method
hvap	56.83	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	2.111		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1538.00		NIST Webbook
rinpol	1538.00		NIST Webbook
tb	624.54	K	Joback Method
tc	847.15	K	Joback Method
tf	394.68	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.54	J/mol×K	624.54	Joback Method
cpg	470.72	J/mol×K	661.64	Joback Method
cpg	485.96	J/mol×K	698.74	Joback Method
cpg	500.39	J/mol×K	735.84	Joback Method
cpg	514.15	J/mol×K	772.95	Joback Method
cpg	527.37	J/mol×K	810.05	Joback Method
cpg	540.16	J/mol×K	847.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R329481&Units=SI
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

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