Cyclopropanecarboxylic acid, trans-2-phenyl-, but-3-yn-2-yl ester

Inchi: InChI=1S/C14H14O2/c1-3-10(2)16-14(15)13-9-12(13)11-7-5-4-6-8-11/h1,4-8,10,12-13H,

InchiKey: IOIWVCMKWWNHQJ-UHFFFAOYSA-N

Formula: C14H14O2

SMILES: C#CC(C)OC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 214.26

Physical Properties

Property code	Value	Unit	Source
gf	219.16	kJ/mol	Joback Method
hf	-1.48	kJ/mol	Joback Method
hfus	27.50	kJ/mol	Joback Method
hvap	57.26	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.355		Crippen Method
mcvol	172.340	ml/mol	McGowan Method
pc	2679.08	kPa	Joback Method
rinpol	1628.00		NIST Webbook
rinpol	1628.00		NIST Webbook
tb	614.44	K	Joback Method
tc	847.37	K	Joback Method
tf	391.79	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.86	J/mol×K	614.44	Joback Method
cpg	455.57	J/mol×K	653.26	Joback Method
cpg	471.07	J/mol×K	692.08	Joback Method
cpg	485.44	J/mol×K	730.90	Joback Method
cpg	498.74	J/mol×K	769.72	Joback Method
cpg	511.07	J/mol×K	808.54	Joback Method
cpg	522.48	J/mol×K	847.37	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=U406834&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
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