Cyclopropanecarboxylic acid, trans-2-phenyl-, hex-4-yn-3-yl ester

Inchi: InChI=1S/C16H18O2/c1-3-8-13(4-2)18-16(17)15-11-14(15)12-9-6-5-7-10-12/h5-7,9-10,1

InchiKey: PRNMSQDOGMHWDP-UHFFFAOYSA-N

Formula: C16H18O2

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

Mol. weight [g/mol]: 242.31

Physical Properties

Property code	Value	Unit	Source
gf	215.73	kJ/mol	Joback Method
hf	-62.36	kJ/mol	Joback Method
hfus	32.83	kJ/mol	Joback Method
hvap	64.01	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.135		Crippen Method
mcvol	200.520	ml/mol	McGowan Method
pc	2241.88	kPa	Joback Method
rinpol	1886.00		NIST Webbook
rinpol	1886.00		NIST Webbook
tb	679.08	K	Joback Method
tc	913.19	K	Joback Method
tf	473.46	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.60	J/mol×K	679.08	Joback Method
cpg	562.62	J/mol×K	718.10	Joback Method
cpg	579.38	J/mol×K	757.12	Joback Method
cpg	594.95	J/mol×K	796.13	Joback Method
cpg	609.40	J/mol×K	835.15	Joback Method
cpg	622.79	J/mol×K	874.17	Joback Method
cpg	635.20	J/mol×K	913.19	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=U406908&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