Cyclopropanecarboxylic acid, trans-2-phenyl-, 2,7-dimethyloct-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C20H24O2/c1-14(2)10-11-17(12-15(3)4)22-20(21)19-13-18(19)16-8-6-5-7-9-16

InchiKey: SVNDBXNNCSRFAN-UHFFFAOYSA-N

Formula: C20H24O2

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

Mol. weight [g/mol]: 296.40

Physical Properties

Property code	Value	Unit	Source
gf	326.26	kJ/mol	Joback Method
hf	-34.56	kJ/mol	Joback Method
hfus	37.08	kJ/mol	Joback Method
hvap	71.94	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.328		Crippen Method
mcvol	252.580	ml/mol	McGowan Method
pc	1678.28	kPa	Joback Method
rinpol	2118.00		NIST Webbook
rinpol	2118.00		NIST Webbook
tb	766.72	K	Joback Method
tc	996.11	K	Joback Method
tf	487.82	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.07	J/mol×K	766.72	Joback Method
cpg	759.97	J/mol×K	804.95	Joback Method
cpg	777.54	J/mol×K	843.18	Joback Method
cpg	793.89	J/mol×K	881.41	Joback Method
cpg	809.10	J/mol×K	919.64	Joback Method
cpg	823.24	J/mol×K	957.88	Joback Method
cpg	836.42	J/mol×K	996.11	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=U406911&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