Cyclopropanecarboxylic acid, trans-2-phenyl-, tridec-2-yn-1-yl ester

Inchi: InChI=1S/C23H32O2/c1-2-3-4-5-6-7-8-9-10-11-15-18-25-23(24)22-19-21(22)20-16-13-12

InchiKey: KXPCSKONBZEVBF-UHFFFAOYSA-N

Formula: C23H32O2

SMILES: CCCCCCCCCCC#CCOC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	277.11	kJ/mol	Joback Method
hf	-201.56	kJ/mol	Joback Method
hfus	54.48	kJ/mol	Joback Method
hvap	79.98	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.868		Crippen Method
mcvol	299.150	ml/mol	McGowan Method
pc	1282.83	kPa	Joback Method
rinpol	2698.00		NIST Webbook
rinpol	2698.00		NIST Webbook
tb	839.68	K	Joback Method
tc	1050.03	K	Joback Method
tf	567.35	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.12	J/mol×K	839.68	Joback Method
cpg	961.98	J/mol×K	874.74	Joback Method
cpg	979.66	J/mol×K	909.80	Joback Method
cpg	996.22	J/mol×K	944.86	Joback Method
cpg	1011.74	J/mol×K	979.91	Joback Method
cpg	1026.29	J/mol×K	1014.97	Joback Method
cpg	1039.93	J/mol×K	1050.03	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406913&Units=SI

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