Cyclopropanecarboxylic acid, trans-2-phenyl-, pent-2-yl ester

Inchi: InChI=1S/C15H20O2/c1-3-7-11(2)17-15(16)14-10-13(14)12-8-5-4-6-9-12/h4-6,8-9,11,13-

InchiKey: OMSLENHFZKYCNX-UHFFFAOYSA-N

Formula: C15H20O2

SMILES: CCCC(C)OC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	4.51	kJ/mol	Joback Method
hf	-314.02	kJ/mol	Joback Method
hfus	27.12	kJ/mol	Joback Method
hvap	59.63	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.522		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1718.00		NIST Webbook
rinpol	1718.00		NIST Webbook
tb	647.20	K	Joback Method
tc	861.24	K	Joback Method
tf	356.09	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.37	J/mol×K	647.20	Joback Method
cpg	552.48	J/mol×K	682.87	Joback Method
cpg	569.44	J/mol×K	718.55	Joback Method
cpg	585.31	J/mol×K	754.22	Joback Method
cpg	600.12	J/mol×K	789.89	Joback Method
cpg	613.95	J/mol×K	825.57	Joback Method
cpg	626.85	J/mol×K	861.24	Joback Method
dvisc	0.0022326	Pa×s	356.09	Joback Method

dvisc	0.0013939	Pa×s	404.61	Joback Method
dvisc	0.0009627	Pa×s	453.13	Joback Method
dvisc	0.0007142	Pa×s	501.65	Joback Method
dvisc	0.0005585	Pa×s	550.16	Joback Method
dvisc	0.0004545	Pa×s	598.68	Joback Method
dvisc	0.0003815	Pa×s	647.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406879&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
dvisc:	Dynamic viscosity
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