Cyclopropanecarboxylic acid, trans-2-phenyl-, 3-methylbut-2-yl ester

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

InchiKey: ZUODJYREEXRIQB-UHFFFAOYSA-N

Formula: C15H20O2

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

Mol. weight [g/mol]: 232.32

Physical Properties

Property code	Value	Unit	Source
gf	2.07	kJ/mol	Joback Method
hf	-319.30	kJ/mol	Joback Method
hfus	23.59	kJ/mol	Joback Method
hvap	59.24	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.378		Crippen Method
mcvol	195.030	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1709.00		NIST Webbook
rinpol	1709.00		NIST Webbook
tb	646.76	K	Joback Method
tc	865.01	K	Joback Method
tf	341.09	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	534.81	J/mol×K	646.76	Joback Method
cpg	553.32	J/mol×K	683.14	Joback Method
cpg	570.62	J/mol×K	719.51	Joback Method
cpg	586.77	J/mol×K	755.89	Joback Method
cpg	601.82	J/mol×K	792.26	Joback Method
cpg	615.84	J/mol×K	828.64	Joback Method
cpg	628.88	J/mol×K	865.01	Joback Method
dvisc	0.0025930	Pa×s	341.09	Joback Method

dvisc	0.0015000	Pa×s	392.04	Joback Method
dvisc	0.0009842	Pa×s	442.98	Joback Method
dvisc	0.0007044	Pa×s	493.93	Joback Method
dvisc	0.0005366	Pa×s	544.87	Joback Method
dvisc	0.0004283	Pa×s	595.82	Joback Method
dvisc	0.0003542	Pa×s	646.76	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=U406835&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
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