Cyclopropanecarboxylic acid, trans-2-phenyl-, 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C15H18O2/c1-11(2)8-9-17-15(16)14-10-13(14)12-6-4-3-5-7-12/h3-8,13-14H,9-

InchiKey: HSALSWZNXPWFEA-UHFFFAOYSA-N

Formula: C15H18O2

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

Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	78.62	kJ/mol	Joback Method
hf	-201.31	kJ/mol	Joback Method
hfus	29.53	kJ/mol	Joback Method
hvap	60.06	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.299		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	1830.00		NIST Webbook
tb	651.68	K	Joback Method
tc	873.69	K	Joback Method
tf	352.05	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.19	J/mol×K	651.68	Joback Method
cpg	529.69	J/mol×K	688.68	Joback Method
cpg	546.01	J/mol×K	725.68	Joback Method
cpg	561.23	J/mol×K	762.69	Joback Method
cpg	575.43	J/mol×K	799.69	Joback Method
cpg	588.67	J/mol×K	836.69	Joback Method
cpg	601.04	J/mol×K	873.69	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=U406837&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