Cyclopropanecarboxylic acid, trans-2-phenyl-, 3-methylphenyl ester

Inchi: InChI=1S/C17H16O2/c1-12-6-5-9-14(10-12)19-17(18)16-11-15(16)13-7-3-2-4-8-13/h2-10

InchiKey: LSHKQCOXYXCMSB-UHFFFAOYSA-N

Formula: C17H16O2

SMILES: Cc1cccc(OC(=O)C2CC2c2ccccc2)c1

Mol. weight [g/mol]: 252.31

Physical Properties

Property code	Value	Unit	Source
gf	126.57	kJ/mol	Joback Method
hf	-124.96	kJ/mol	Joback Method
hfus	29.47	kJ/mol	Joback Method
hvap	67.41	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.704		Crippen Method
mcvol	199.450	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	2145.00		NIST Webbook
rinpol	2145.00		NIST Webbook
tb	725.06	K	Joback Method
tc	969.46	K	Joback Method
tf	432.57	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.62	J/mol×K	725.06	Joback Method
cpg	631.33	J/mol×K	928.73	Joback Method
cpg	619.19	J/mol×K	887.99	Joback Method
cpg	605.93	J/mol×K	847.26	Joback Method
cpg	591.48	J/mol×K	806.53	Joback Method
cpg	575.74	J/mol×K	765.79	Joback Method
cpg	642.47	J/mol×K	969.46	Joback Method
dvisc	0.0003737	Pa×s	725.06	Joback Method

dvisc	0.0004351	Pa×s	676.31	Joback Method
dvisc	0.0005188	Pa×s	627.56	Joback Method
dvisc	0.0006372	Pa×s	578.81	Joback Method
dvisc	0.0008127	Pa×s	530.07	Joback Method
dvisc	0.0010890	Pa×s	481.32	Joback Method
dvisc	0.0015587	Pa×s	432.57	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=U406882&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