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

Inchi: InChI=1S/C17H24O2/c1-3-4-6-9-13(2)19-17(18)16-12-15(16)14-10-7-5-8-11-14/h5,7-8,1

InchiKey: SINSXGWSOOGAOP-UHFFFAOYSA-N

Formula: C17H24O2

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

Mol. weight [g/mol]: 260.37

Physical Properties

Property code	Value	Unit	Source
gf	21.35	kJ/mol	Joback Method
hf	-355.30	kJ/mol	Joback Method
hfus	32.30	kJ/mol	Joback Method
hvap	64.08	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.302		Crippen Method
mcvol	223.210	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	1903.00		NIST Webbook
rinpol	1903.00		NIST Webbook
tb	692.96	K	Joback Method
tc	900.69	K	Joback Method
tf	378.63	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	642.91	J/mol×K	692.96	Joback Method
cpg	725.11	J/mol×K	866.06	Joback Method
cpg	710.76	J/mol×K	831.44	Joback Method
cpg	695.43	J/mol×K	796.82	Joback Method
cpg	679.04	J/mol×K	762.20	Joback Method
cpg	661.56	J/mol×K	727.58	Joback Method
cpg	738.52	J/mol×K	900.69	Joback Method
dvisc	0.0003267	Pa×s	692.96	Joback Method

dvisc	0.0003940	Pa×s	640.57	Joback Method
dvisc	0.0004913	Pa×s	588.18	Joback Method
dvisc	0.0006396	Pa×s	535.80	Joback Method
dvisc	0.0008817	Pa×s	483.41	Joback Method
dvisc	0.0013142	Pa×s	431.02	Joback Method
dvisc	0.0021874	Pa×s	378.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406840&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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