Cyclopropanecarboxylic acid, trans-2-phenyl-, undecyl ester

Inchi: InChI=1S/C21H32O2/c1-2-3-4-5-6-7-8-9-13-16-23-21(22)20-17-19(20)18-14-11-10-12-15

InchiKey: YIWYPAZHWDXXCJ-UHFFFAOYSA-N

Formula: C21H32O2

SMILES: CCCCCCCCCCCOC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 316.48

Physical Properties

Property code	Value	Unit	Source
gf	57.47	kJ/mol	Joback Method
hf	-432.58	kJ/mol	Joback Method
hfus	46.18	kJ/mol	Joback Method
hvap	73.38	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.864		Crippen Method
mcvol	279.570	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	2444.00		NIST Webbook
rinpol	2444.00		NIST Webbook
tb	784.92	K	Joback Method
tc	982.86	K	Joback Method
tf	438.71	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.75	J/mol×K	784.92	Joback Method
cpg	891.79	J/mol×K	817.91	Joback Method
cpg	909.70	J/mol×K	850.90	Joback Method
cpg	926.53	J/mol×K	883.89	Joback Method
cpg	942.36	J/mol×K	916.88	Joback Method
cpg	957.23	J/mol×K	949.87	Joback Method
cpg	971.20	J/mol×K	982.86	Joback Method
dvisc	0.0016721	Pa×s	438.71	Joback Method

dvisc	0.0010038	Pa×s	496.41	Joback Method
dvisc	0.0006702	Pa×s	554.11	Joback Method
dvisc	0.0004829	Pa×s	611.81	Joback Method
dvisc	0.0003681	Pa×s	669.52	Joback Method
dvisc	0.0002930	Pa×s	727.22	Joback Method
dvisc	0.0002412	Pa×s	784.92	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=U406002&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