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

Inchi: InChI=1S/C23H36O2/c1-3-5-6-7-8-9-10-14-17-20(4-2)25-23(24)22-18-21(22)19-15-12-11

InchiKey: KWXCYZUYUNIGAK-UHFFFAOYSA-N

Formula: C23H36O2

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

Mol. weight [g/mol]: 344.53

Physical Properties

Property code	Value	Unit	Source
gf	71.87	kJ/mol	Joback Method
hf	-479.14	kJ/mol	Joback Method
hfus	47.84	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.643		Crippen Method
mcvol	307.750	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	830.24	K	Joback Method
tc	1030.19	K	Joback Method
tf	446.25	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.90	J/mol×K	830.24	Joback Method
cpg	1013.46	J/mol×K	863.57	Joback Method
cpg	1031.82	J/mol×K	896.89	Joback Method
cpg	1049.07	J/mol×K	930.22	Joback Method
cpg	1065.26	J/mol×K	963.54	Joback Method
cpg	1080.47	J/mol×K	996.87	Joback Method
cpg	1094.75	J/mol×K	1030.19	Joback Method
dvisc	0.0016481	Pa×s	446.25	Joback Method

dvisc	0.0009001	Pa×s	510.25	Joback Method
dvisc	0.0005625	Pa×s	574.25	Joback Method
dvisc	0.0003863	Pa×s	638.25	Joback Method
dvisc	0.0002841	Pa×s	702.24	Joback Method
dvisc	0.0002199	Pa×s	766.24	Joback Method
dvisc	0.0001771	Pa×s	830.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406250&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

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

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