

Cyclopropanecarboxylic acid, trans-2-phenyl-, tridec-5-yl ester

Inchi:	InChI=1S/C23H36O2/c1-3-5-7-8-9-13-17-20(16-6-4-2)25-23(24)22-18-21(22)19-14-11-10
InchiKey:	RVRSOFDORKXKFK-UHFFFAOYSA-N
Formula:	C23H36O2
SMILES:	CCCCCCCCC(CCCC)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	2454.00		NIST Webbook
rinpol	2454.00		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/molxK	830.24	Joback Method
cpg	1080.47	J/molxK	996.87	Joback Method
cpg	1065.26	J/molxK	963.54	Joback Method
cpg	1049.07	J/molxK	930.22	Joback Method
cpg	1031.82	J/molxK	896.89	Joback Method
cpg	1013.46	J/molxK	863.57	Joback Method
cpg	1094.75	J/molxK	1030.19	Joback Method
dvisc	0.0001771	Paxs	830.24	Joback Method

dvisc	0.0002199	Paxs	766.24	Joback Method
dvisc	0.0002841	Paxs	702.24	Joback Method
dvisc	0.0003863	Paxs	638.25	Joback Method
dvisc	0.0005625	Paxs	574.25	Joback Method
dvisc	0.0009001	Paxs	510.25	Joback Method
dvisc	0.0016481	Paxs	446.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406252&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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