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

Inchi: InChI=1S/C23H36O2/c1-2-3-4-5-6-7-8-9-10-11-15-18-25-23(24)22-19-21(22)20-16-13-12

InchiKey: VNAWSZRMBXWLRQ-UHFFFAOYSA-N

Formula: C23H36O2

SMILES: CCCCCCCCCCCCCOC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 344.53

Physical Properties

Property code	Value	Unit	Source
gf	74.31	kJ/mol	Joback Method
hf	-473.86	kJ/mol	Joback Method
hfus	51.36	kJ/mol	Joback Method
hvap	77.83	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.644		Crippen Method
mcvol	307.750	ml/mol	McGowan Method
pc	1147.54	kPa	Joback Method
rinpol	2657.00		NIST Webbook
rinpol	2657.00		NIST Webbook
tb	830.68	K	Joback Method
tc	1028.86	K	Joback Method
tf	461.25	K	Joback Method
vc	1.196	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	993.43	J/mol×K	830.68	Joback Method
cpg	1012.82	J/mol×K	863.71	Joback Method
cpg	1031.05	J/mol×K	896.74	Joback Method
cpg	1048.19	J/mol×K	929.77	Joback Method
cpg	1064.31	J/mol×K	962.80	Joback Method
cpg	1079.46	J/mol×K	995.83	Joback Method
cpg	1093.72	J/mol×K	1028.86	Joback Method
dvisc	0.0014841	Pa×s	461.25	Joback Method

dvisc	0.0008650	Pa×s	522.82	Joback Method
dvisc	0.0005649	Pa×s	584.39	Joback Method
dvisc	0.0004001	Pa×s	645.96	Joback Method
dvisc	0.0003010	Pa×s	707.54	Joback Method
dvisc	0.0002369	Pa×s	769.11	Joback Method
dvisc	0.0001932	Pa×s	830.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406004&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