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

Inchi: InChI=1S/C22H34O2/c1-2-3-4-5-6-7-8-9-10-14-17-24-22(23)21-18-20(21)19-15-12-11-13

InchiKey: JZJYVMZMAIRKBY-UHFFFAOYSA-N

Formula: C22H34O2

SMILES: CCCCCCCCCCCCOC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 330.50

Physical Properties

Property code	Value	Unit	Source
gf	65.89	kJ/mol	Joback Method
hf	-453.22	kJ/mol	Joback Method
hfus	48.77	kJ/mol	Joback Method
hvap	75.60	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	6.254		Crippen Method
mcvol	293.660	ml/mol	McGowan Method
pc	1225.98	kPa	Joback Method
rinpol	2553.00		NIST Webbook
rinpol	2553.00		NIST Webbook
tb	807.80	K	Joback Method
tc	1005.54	K	Joback Method
tf	449.98	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	932.68	J/mol×K	807.80	Joback Method
cpg	951.89	J/mol×K	840.76	Joback Method
cpg	969.95	J/mol×K	873.71	Joback Method
cpg	986.94	J/mol×K	906.67	Joback Method
cpg	1002.91	J/mol×K	939.63	Joback Method
cpg	1017.92	J/mol×K	972.58	Joback Method
cpg	1032.03	J/mol×K	1005.54	Joback Method
dvisc	0.0015806	Pa×s	449.98	Joback Method

dvisc	0.0009347	Pa×s	509.62	Joback Method
dvisc	0.0006170	Pa×s	569.25	Joback Method
dvisc	0.0004407	Pa×s	628.89	Joback Method
dvisc	0.0003337	Pa×s	688.53	Joback Method
dvisc	0.0002641	Pa×s	748.16	Joback Method
dvisc	0.0002164	Pa×s	807.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406003&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