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

Inchi: InChI=1S/C16H22O2/c1-2-3-4-8-11-18-16(17)15-12-14(15)13-9-6-5-7-10-13/h5-7,9-10,1

InchiKey: AITACQSZDPZEDG-UHFFFAOYSA-N

Formula: C16H22O2

SMILES: CCCCCCOC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 246.34

Physical Properties

Property code	Value	Unit	Source
gf	15.37	kJ/mol	Joback Method
hf	-329.38	kJ/mol	Joback Method
hfus	33.23	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	3.914		Crippen Method
mcvol	209.120	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	1919.00		NIST Webbook
rinpol	1919.00		NIST Webbook
tb	670.52	K	Joback Method
tc	877.44	K	Joback Method
tf	382.36	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.57	J/mol×K	670.52	Joback Method
cpg	667.26	J/mol×K	842.95	Joback Method
cpg	653.32	J/mol×K	808.46	Joback Method
cpg	638.44	J/mol×K	773.98	Joback Method
cpg	622.55	J/mol×K	739.49	Joback Method
cpg	605.61	J/mol×K	705.01	Joback Method
cpg	680.30	J/mol×K	877.44	Joback Method
dvisc	0.0003824	Pa×s	670.52	Joback Method

dvisc	0.0004521	Pa×s	622.49	Joback Method
dvisc	0.0005497	Pa×s	574.47	Joback Method
dvisc	0.0006926	Pa×s	526.44	Joback Method
dvisc	0.0009141	Pa×s	478.41	Joback Method
dvisc	0.0012835	Pa×s	430.39	Joback Method
dvisc	0.0019626	Pa×s	382.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405998&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