Cyclopropanecarboxylic acid, trans-2-phenyl-, 4-methyl-2-pentyl ester

Inchi: InChI=1S/C16H22O2/c1-11(2)9-12(3)18-16(17)15-10-14(15)13-7-5-4-6-8-13/h4-8,11-12,
InchiKey: FAYWPWSOIKTNCR-UHFFFAOYSA-N
Formula: C16H22O2
SMILES: CC(C)CC(C)OC(=O)C1CC1c1ccccc1
Mol. weight [g/mol]: 246.34

Physical Properties

Property code	Value	Unit	Source
gf	10.49	kJ/mol	Joback Method
hf	-339.94	kJ/mol	Joback Method
hfus	26.18	kJ/mol	Joback Method
hvap	61.47	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.768		Crippen Method
mcvol	209.120	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
tb	669.64	K	Joback Method
tc	884.28	K	Joback Method
tf	352.36	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.48	J/mol×K	669.64	Joback Method
cpg	607.27	J/mol×K	705.41	Joback Method
cpg	624.84	J/mol×K	741.19	Joback Method
cpg	641.27	J/mol×K	776.96	Joback Method
cpg	656.59	J/mol×K	812.73	Joback Method
cpg	670.88	J/mol×K	848.51	Joback Method
cpg	684.20	J/mol×K	884.28	Joback Method
dvisc	0.0025727	Pa×s	352.36	Joback Method

dvisc	0.0014594	Pa×s	405.24	Joback Method
dvisc	0.0009437	Pa×s	458.12	Joback Method
dvisc	0.0006678	Pa×s	511.00	Joback Method
dvisc	0.0005042	Pa×s	563.88	Joback Method
dvisc	0.0003995	Pa×s	616.76	Joback Method
dvisc	0.0003284	Pa×s	669.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405995&Units=SI

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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