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

Inchi: InChI=1S/C18H26O2/c1-2-3-4-5-6-10-13-20-18(19)17-14-16(17)15-11-8-7-9-12-15/h7-9,
InchiKey: ANWXAJQWYWWNGX-UHFFFAOYSA-N
Formula: C18H26O2
SMILES: CCCCCCCCOC(=O)C1CC1c1ccccc1
Mol. weight [g/mol]: 274.40

Physical Properties

Property code	Value	Unit	Source
gf	32.21	kJ/mol	Joback Method
hf	-370.66	kJ/mol	Joback Method
hfus	38.41	kJ/mol	Joback Method
hvap	66.70	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.694		Crippen Method
mcvol	237.300	ml/mol	McGowan Method
pc	1636.45	kPa	Joback Method
rinpol	2128.00		NIST Webbook
rinpol	2128.00		NIST Webbook
tb	716.28	K	Joback Method
tc	918.20	K	Joback Method
tf	404.90	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.47	J/mol×K	716.28	Joback Method
cpg	716.99	J/mol×K	749.93	Joback Method
cpg	734.39	J/mol×K	783.59	Joback Method
cpg	750.74	J/mol×K	817.24	Joback Method
cpg	766.08	J/mol×K	850.89	Joback Method
cpg	780.47	J/mol×K	884.54	Joback Method
cpg	793.96	J/mol×K	918.20	Joback Method
dvisc	0.0018915	Pa×s	404.90	Joback Method

dvisc	0.0011927	Pa×s	456.80	Joback Method
dvisc	0.0008263	Pa×s	508.69	Joback Method
dvisc	0.0006127	Pa×s	560.59	Joback Method
dvisc	0.0004779	Pa×s	612.49	Joback Method
dvisc	0.0003875	Pa×s	664.38	Joback Method
dvisc	0.0003240	Pa×s	716.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405999&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

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