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

Inchi: InChI=1S/C16H14O2/c17-16(18-13-9-5-2-6-10-13)15-11-14(15)12-7-3-1-4-8-12/h1-10,14

InchiKey: RFWVVXSKWXDEGN-UHFFFAOYSA-N

Formula: C16H14O2

SMILES: O=C(Oc1ccccc1)C1CC1c1ccccc1

Mol. weight [g/mol]: 238.28

Physical Properties

Property code	Value	Unit	Source
gf	127.78	kJ/mol	Joback Method
hf	-92.85	kJ/mol	Joback Method
hfus	27.27	kJ/mol	Joback Method
hvap	64.52	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.396		Crippen Method
mcvol	185.360	ml/mol	McGowan Method
pc	2632.55	kPa	Joback Method
rinpol	2036.00		NIST Webbook
rinpol	2036.00		NIST Webbook
tb	697.20	K	Joback Method
tc	946.14	K	Joback Method
tf	408.78	K	Joback Method
vc	0.696	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.17	J/mol×K	697.20	Joback Method
cpg	523.22	J/mol×K	738.69	Joback Method
cpg	538.83	J/mol×K	780.18	Joback Method
cpg	553.10	J/mol×K	821.67	Joback Method
cpg	566.14	J/mol×K	863.16	Joback Method
cpg	578.04	J/mol×K	904.65	Joback Method
cpg	588.91	J/mol×K	946.14	Joback Method
dvisc	0.0018090	Pa×s	408.78	Joback Method

dvisc	0.0012332	Pa×s	456.85	Joback Method
dvisc	0.0009043	Pa×s	504.92	Joback Method
dvisc	0.0006999	Pa×s	552.99	Joback Method
dvisc	0.0005643	Pa×s	601.06	Joback Method
dvisc	0.0004697	Pa×s	649.13	Joback Method
dvisc	0.0004010	Pa×s	697.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406881&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