Cyclopropanecarboxylic acid, trans-2-phenyl-, 3-chlorophenyl ester

Inchi: InChI=1S/C16H13ClO2/c17-12-7-4-8-13(9-12)19-16(18)15-10-14(15)11-5-2-1-3-6-11/h1-

InchiKey: ZIIUPZXWJIGURA-UHFFFAOYSA-N

Formula: C16H13ClO2

SMILES: O=C(Oc1cccc(Cl)c1)C1CC1c1ccccc1

Mol. weight [g/mol]: 272.73

Physical Properties

Property code	Value	Unit	Source
gf	106.22	kJ/mol	Joback Method
hf	-120.06	kJ/mol	Joback Method
hfus	31.08	kJ/mol	Joback Method
hvap	69.57	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	4.049		Crippen Method
mcvol	197.600	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	2188.00		NIST Webbook
rinpol	2188.00		NIST Webbook
tb	739.61	K	Joback Method
tc	991.44	K	Joback Method
tf	451.22	K	Joback Method
vc	0.745	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.87	J/mol×K	739.61	Joback Method
cpg	595.33	J/mol×K	949.47	Joback Method
cpg	584.71	J/mol×K	907.50	Joback Method
cpg	573.05	J/mol×K	865.52	Joback Method
cpg	560.26	J/mol×K	823.55	Joback Method
cpg	546.23	J/mol×K	781.58	Joback Method
cpg	605.01	J/mol×K	991.44	Joback Method
dvisc	0.0003911	Pa×s	739.61	Joback Method

dvisc	0.0004549	Pa×s	691.55	Joback Method
dvisc	0.0005413	Pa×s	643.48	Joback Method
dvisc	0.0006623	Pa×s	595.41	Joback Method
dvisc	0.0008396	Pa×s	547.35	Joback Method
dvisc	0.0011142	Pa×s	499.29	Joback Method
dvisc	0.0015704	Pa×s	451.22	Joback Method

Sources

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=U406844&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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