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

Inchi: InChI=1S/C12H12Cl2O2/c13-11(14)7-16-12(15)10-6-9(10)8-4-2-1-3-5-8/h1-5,9-11H,6-7H

InchiKey: UEBPXVAGGLVLOG-UHFFFAOYSA-N

Formula: C12H12Cl2O2

SMILES: O=C(OCC(Cl)Cl)C1CC1c1ccccc1

Mol. weight [g/mol]: 259.13

Physical Properties

Property code	Value	Unit	Source
gf	-44.61	kJ/mol	Joback Method
hf	-283.58	kJ/mol	Joback Method
hfus	27.74	kJ/mol	Joback Method
hvap	61.72	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.137		Crippen Method
mcvol	177.240	ml/mol	McGowan Method
pc	2597.78	kPa	Joback Method
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
tb	653.42	K	Joback Method
tc	886.05	K	Joback Method
tf	382.12	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.08	J/mol×K	653.42	Joback Method
cpg	450.42	J/mol×K	692.19	Joback Method
cpg	463.67	J/mol×K	730.96	Joback Method
cpg	475.90	J/mol×K	769.74	Joback Method
cpg	487.16	J/mol×K	808.51	Joback Method
cpg	497.54	J/mol×K	847.28	Joback Method
cpg	507.07	J/mol×K	886.05	Joback Method
dvisc	0.0022507	Pa×s	382.12	Joback Method

dvisc	0.0015027	Pa×s	427.34	Joback Method
dvisc	0.0010839	Pa×s	472.55	Joback Method
dvisc	0.0008277	Pa×s	517.77	Joback Method
dvisc	0.0006601	Pa×s	562.99	Joback Method
dvisc	0.0005444	Pa×s	608.20	Joback Method
dvisc	0.0004611	Pa×s	653.42	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=U406838&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