Cyclopropanecarboxylic acid, trans-2-phenyl-, 8-chlorooctyl ester

Inchi: InChI=1S/C18H25ClO2/c19-12-8-3-1-2-4-9-13-21-18(20)17-14-16(17)15-10-6-5-7-11-15/

InchiKey: BIAZODDACMIMPI-UHFFFAOYSA-N

Formula: C18H25ClO2

SMILES: O=C(OCCCCCCCCCl)C1CC1c1ccccc1

Mol. weight [g/mol]: 308.84

Physical Properties

Property code	Value	Unit	Source
gf	20.28	kJ/mol	Joback Method
hf	-386.40	kJ/mol	Joback Method
hfus	42.61	kJ/mol	Joback Method
hvap	71.08	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.913		Crippen Method
mcvol	249.540	ml/mol	McGowan Method
pc	1588.54	kPa	Joback Method
rinpol	2449.00		NIST Webbook
tb	753.71	K	Joback Method
tc	959.25	K	Joback Method
tf	434.82	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	729.26	J/mol×K	753.71	Joback Method
cpg	746.55	J/mol×K	787.97	Joback Method
cpg	762.75	J/mol×K	822.22	Joback Method
cpg	777.92	J/mol×K	856.48	Joback Method
cpg	792.13	J/mol×K	890.74	Joback Method
cpg	805.42	J/mol×K	925.00	Joback Method
cpg	817.86	J/mol×K	959.25	Joback Method
dvisc	0.0017795	Pa×s	434.82	Joback Method
dvisc	0.0011294	Pa×s	487.97	Joback Method

dvisc	0.0007838	Pa×s	541.12	Joback Method
dvisc	0.0005807	Pa×s	594.26	Joback Method
dvisc	0.0004519	Pa×s	647.41	Joback Method
dvisc	0.0003654	Pa×s	700.56	Joback Method
dvisc	0.0003044	Pa×s	753.71	Joback Method

Sources

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=U406847&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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