

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

Inchi:	InChI=1S/C13H16O2/c1-9(2)15-13(14)12-8-11(12)10-6-4-3-5-7-10/h3-7,9,11-12H,8H2,1-
InchiKey:	FDQAUEOMWMJQSX-UHFFFAOYSA-N
Formula:	C13H16O2
SMILES:	CC(C)OC(=O)C1CC1c1ccccc1
Mol. weight [g/mol]:	204.26

Physical Properties

Property code	Value	Unit	Source
gf	-12.33	kJ/mol	Joback Method
hf	-272.74	kJ/mol	Joback Method
hfus	21.94	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.742		Crippen Method
mvol	166.850	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1539.00		NIST Webbook
tb	601.44	K	Joback Method
tc	823.08	K	Joback Method
tf	333.55	K	Joback Method
vc	0.629	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.08	J/molxK	601.44	Joback Method
cpg	448.38	J/molxK	638.38	Joback Method
cpg	464.54	J/molxK	675.32	Joback Method
cpg	479.62	J/molxK	712.26	Joback Method
cpg	493.67	J/molxK	749.20	Joback Method
cpg	506.74	J/molxK	786.14	Joback Method
cpg	518.89	J/molxK	823.08	Joback Method
dvisc	0.0021670	Paxs	333.55	Joback Method

dvisc	0.0014119	Paxs	378.20	Joback Method
dvisc	0.0010070	Paxs	422.85	Joback Method
dvisc	0.0007661	Paxs	467.50	Joback Method
dvisc	0.0006113	Paxs	512.14	Joback Method
dvisc	0.0005057	Paxs	556.79	Joback Method
dvisc	0.0004304	Paxs	601.44	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=U405992&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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