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

Inchi: InChI=1S/C14H18O2/c1-10(2)9-16-14(15)13-8-12(13)11-6-4-3-5-7-11/h3-7,10,12-13H,8-

InchiKey: DRBACORAXKIPLB-UHFFFAOYSA-N

Formula: C14H18O2

SMILES: CC(C)COC(=O)C1CC1c1ccccc1

Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
gf	-3.91	kJ/mol	Joback Method
hf	-293.38	kJ/mol	Joback Method
hfus	24.53	kJ/mol	Joback Method
hvap	57.41	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.989		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
pc	2311.39	kPa	Joback Method
rinpol	1667.00		NIST Webbook
rinpol	1667.00		NIST Webbook
tb	624.32	K	Joback Method
tc	842.02	K	Joback Method
tf	344.82	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.03	J/mol×K	624.32	Joback Method
cpg	559.84	J/mol×K	805.74	Joback Method
cpg	546.36	J/mol×K	769.45	Joback Method
cpg	531.89	J/mol×K	733.17	Joback Method
cpg	516.38	J/mol×K	696.89	Joback Method
cpg	499.77	J/mol×K	660.60	Joback Method
cpg	572.40	J/mol×K	842.02	Joback Method
dvisc	0.0004071	Pa×s	624.32	Joback Method

dvisc	0.0004818	Pa×s	577.74	Joback Method
dvisc	0.0005874	Pa×s	531.15	Joback Method
dvisc	0.0007438	Pa×s	484.57	Joback Method
dvisc	0.0009904	Pa×s	437.99	Joback Method
dvisc	0.0014119	Pa×s	391.40	Joback Method
dvisc	0.0022150	Pa×s	344.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405993&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

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