Cyclobutanecarboxylic acid, 2-isopropoxyohenyl ester

Inchi: InChI=1S/C14H18O3/c1-10(2)16-12-8-3-4-9-13(12)17-14(15)11-6-5-7-11/h3-4,8-11H,5-7

InchiKey: LGYNTCSGORWHHN-UHFFFAOYSA-N

Formula: C14H18O3

SMILES: CC(C)Oc1ccccc1OC(=O)C1CCC1

Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
gf	-122.93	kJ/mol	Joback Method
hf	-422.89	kJ/mol	Joback Method
hfus	22.16	kJ/mol	Joback Method
hvap	60.96	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.179		Crippen Method
mcvol	186.810	ml/mol	McGowan Method
pc	2370.28	kPa	Joback Method
rinpol	1656.00		NIST Webbook
tb	660.66	K	Joback Method
tc	883.48	K	Joback Method
tf	380.29	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.95	J/mol×K	660.66	Joback Method
cpg	584.76	J/mol×K	846.34	Joback Method
cpg	571.76	J/mol×K	809.20	Joback Method
cpg	557.72	J/mol×K	772.07	Joback Method
cpg	542.59	J/mol×K	734.93	Joback Method
cpg	526.34	J/mol×K	697.80	Joback Method
cpg	596.75	J/mol×K	883.48	Joback Method
dvisc	0.0002106	Pa×s	660.66	Joback Method
dvisc	0.0002602	Pa×s	613.93	Joback Method

dvisc	0.0003330	Pa×s	567.20	Joback Method
dvisc	0.0004453	Pa×s	520.48	Joback Method
dvisc	0.0006307	Pa×s	473.75	Joback Method
dvisc	0.0009639	Pa×s	427.02	Joback Method
dvisc	0.0016351	Pa×s	380.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299075&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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