4-(1-Propenyl)-phenyl-isobutyrate

Inchi: InChI=1S/C13H16O2/c1-4-5-11-6-8-12(9-7-11)15-13(14)10(2)3/h4-10H,1-3H3/b5-4+
InchiKey: LJEWVBGJLXRKQV-SNAWJCMRSA-N
Formula: C13H16O2
SMILES: CC=Cc1ccc(OC(=O)C(C)C)cc1
Mol. weight [g/mol]: 204.26

Physical Properties

Property code	Value	Unit	Source
gf	5.22	kJ/mol	Joback Method
hf	-219.45	kJ/mol	Joback Method
hfus	22.54	kJ/mol	Joback Method
hvap	56.20	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	3.281		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2393.53	kPa	Joback Method
ripol	2182.00		NIST Webbook
ripol	2182.00		NIST Webbook
ripol	2182.00		NIST Webbook
tb	608.51	K	Joback Method
tc	825.22	K	Joback Method
tf	327.29	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.05	J/mol×K	608.51	Joback Method
cpg	491.15	J/mol×K	789.10	Joback Method
cpg	479.26	J/mol×K	752.98	Joback Method
cpg	466.54	J/mol×K	716.86	Joback Method
cpg	452.95	J/mol×K	680.75	Joback Method
cpg	438.47	J/mol×K	644.63	Joback Method
cpg	502.25	J/mol×K	825.22	Joback Method

dvisc	0.0001316	Pa×s	608.51	Joback Method
dvisc	0.0001707	Pa×s	561.64	Joback Method
dvisc	0.0002323	Pa×s	514.77	Joback Method
dvisc	0.0003361	Pa×s	467.90	Joback Method
dvisc	0.0005281	Pa×s	421.03	Joback Method
dvisc	0.0009292	Pa×s	374.16	Joback Method
dvisc	0.0019222	Pa×s	327.29	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=R418254&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume