4-Oxo-4-phenylbutyric acid, isobutyl ester

Inchi: InChI=1S/C14H18O3/c1-11(2)10-17-14(16)9-8-13(15)12-6-4-3-5-7-12/h3-7,11H,8-10H2,1
InchiKey: JDSNVPCDHHNIPF-UHFFFAOYSA-N
Formula: C14H18O3
SMILES: CC(C)COC(=O)CCC(=O)c1ccccc1
Mol. weight [g/mol]: 234.29

Physical Properties

Property code	Value	Unit	Source
gf	-185.87	kJ/mol	Joback Method
hf	-458.42	kJ/mol	Joback Method
hfus	26.92	kJ/mol	Joback Method
hvap	64.55	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.849		Crippen Method
mcvol	193.370	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1836.00		NIST Webbook
rinpol	1836.00		NIST Webbook
tb	676.12	K	Joback Method
tc	886.75	K	Joback Method
tf	381.05	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.75	J/mol×K	676.12	Joback Method
cpg	529.89	J/mol×K	711.22	Joback Method
cpg	544.07	J/mol×K	746.33	Joback Method
cpg	557.30	J/mol×K	781.43	Joback Method
cpg	569.61	J/mol×K	816.54	Joback Method
cpg	581.04	J/mol×K	851.64	Joback Method
cpg	591.60	J/mol×K	886.75	Joback Method
dvisc	0.0020219	Pa×s	381.05	Joback Method

dvisc	0.0010098	Pa×s	430.23	Joback Method
dvisc	0.0005816	Pa×s	479.41	Joback Method
dvisc	0.0003711	Pa×s	528.59	Joback Method
dvisc	0.0002557	Pa×s	577.76	Joback Method
dvisc	0.0001867	Pa×s	626.94	Joback Method
dvisc	0.0001428	Pa×s	676.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405974&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