2-((Pentan-2-yloxy)carbonyl)benzoic acid

Inchi: InChI=1S/C13H16O4/c1-3-6-9(2)17-13(16)11-8-5-4-7-10(11)12(14)15/h4-5,7-9H,3,6H2,1
InchiKey: MDKPYAGDECEICL-UHFFFAOYSA-N
Formula: C13H16O4
SMILES: CCCC(C)OC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 236.26
CAS: 158703-44-7

Physical Properties

Property code	Value	Unit	Source
gf	-340.74	kJ/mol	Joback Method
hf	-601.48	kJ/mol	Joback Method
hfus	28.03	kJ/mol	Joback Method
hvap	79.66	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	2.730		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2654.29	kPa	Joback Method
rinpol	1842.00		NIST Webbook
tb	750.40	K	Joback Method
tc	953.14	K	Joback Method
tf	443.12	K	Joback Method
vc	0.699	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.58	J/mol×K	750.40	Joback Method
cpg	566.35	J/mol×K	919.35	Joback Method
cpg	557.69	J/mol×K	885.56	Joback Method
cpg	548.30	J/mol×K	851.77	Joback Method
cpg	538.17	J/mol×K	817.98	Joback Method
cpg	527.27	J/mol×K	784.19	Joback Method
cpg	574.30	J/mol×K	953.14	Joback Method
dvisc	0.0000326	Pa×s	750.40	Joback Method

dvisc	0.0000477	Pa×s	699.19	Joback Method
dvisc	0.0000740	Pa×s	647.97	Joback Method
dvisc	0.0001238	Pa×s	596.76	Joback Method
dvisc	0.0002282	Pa×s	545.55	Joback Method
dvisc	0.0004776	Pa×s	494.33	Joback Method
dvisc	0.0011855	Pa×s	443.12	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=C158703447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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