2-((4-Methylpentan-2-yloxy)carbonyl)benzoic acid

Inchi: InChI=1S/C14H18O4/c1-9(2)8-10(3)18-14(17)12-7-5-4-6-11(12)13(15)16/h4-7,9-10H,8H
InchiKey: WBCHJVGWGRPPOT-UHFFFAOYSA-N
Formula: C14H18O4
SMILES: CC(C)CC(C)OC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 250.29
CAS: 856806-35-4

Physical Properties

Property code	Value	Unit	Source
gf	-334.76	kJ/mol	Joback Method
hf	-627.40	kJ/mol	Joback Method
hfus	27.10	kJ/mol	Joback Method
hvap	81.50	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.976		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	1896.00		NIST Webbook
rinpol	1896.00		NIST Webbook
tb	772.84	K	Joback Method
tc	976.87	K	Joback Method
tf	439.39	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.69	J/mol×K	772.84	Joback Method
cpg	581.99	J/mol×K	806.84	Joback Method
cpg	593.43	J/mol×K	840.85	Joback Method
cpg	604.04	J/mol×K	874.85	Joback Method
cpg	613.85	J/mol×K	908.86	Joback Method
cpg	622.87	J/mol×K	942.86	Joback Method
cpg	631.13	J/mol×K	976.87	Joback Method

dvisc	0.0013095	Pa×s	439.39	Joback Method
dvisc	0.0004687	Pa×s	494.97	Joback Method
dvisc	0.0002064	Pa×s	550.54	Joback Method
dvisc	0.0001057	Pa×s	606.12	Joback Method
dvisc	0.0000605	Pa×s	661.69	Joback Method
dvisc	0.0000378	Pa×s	717.26	Joback Method
dvisc	0.0000253	Pa×s	772.84	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=C856806354&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