2-((3-Methylbutan-2-yloxy)carbonyl)benzoic acid

Inchi: InChI=1S/C13H16O4/c1-8(2)9(3)17-13(16)11-7-5-4-6-10(11)12(14)15/h4-9H,1-3H3,(H,14

InchiKey: AJRMLQSJNSDUHW-UHFFFAOYSA-N

Formula: C13H16O4

SMILES: CC(C)C(C)OC(=O)c1ccccc1C(=O)O

Mol. weight [g/mol]: 236.26

CAS: 198284-10-5

Physical Properties

Property code	Value	Unit	Source
gf	-343.18	kJ/mol	Joback Method
hf	-606.76	kJ/mol	Joback Method
hfus	24.51	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.586		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
rinpol	1839.00		NIST Webbook
rinpol	1839.00		NIST Webbook
tb	749.96	K	Joback Method
tc	955.69	K	Joback Method
tf	428.12	K	Joback Method
vc	0.693	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.17	J/mol×K	749.96	Joback Method
cpg	567.52	J/mol×K	921.40	Joback Method
cpg	558.81	J/mol×K	887.11	Joback Method
cpg	549.34	J/mol×K	852.83	Joback Method
cpg	539.09	J/mol×K	818.54	Joback Method
cpg	528.04	J/mol×K	784.25	Joback Method
cpg	575.49	J/mol×K	955.69	Joback Method

dvisc	0.0000301	Pa×s	749.96	Joback Method
dvisc	0.0000450	Pa×s	696.32	Joback Method
dvisc	0.0000721	Pa×s	642.68	Joback Method
dvisc	0.0001257	Pa×s	589.04	Joback Method
dvisc	0.0002452	Pa×s	535.40	Joback Method
dvisc	0.0005548	Pa×s	481.76	Joback Method
dvisc	0.0015402	Pa×s	428.12	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=C198284105&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume