2-((3-Methylbut-3-enyloxy)carbonyl)benzoic acid

Inchi: InChI=1S/C13H14O4/c1-9(2)7-8-17-13(16)11-6-4-3-5-10(11)12(14)15/h3-6H,1,7-8H2,2H

InchiKey: ZCIHYROMGVHDDM-UHFFFAOYSA-N

Formula: C13H14O4

SMILES: C=C(C)CCOC(=O)c1ccccc1C(=O)O

Mol. weight [g/mol]: 234.25

CAS: 113793-37-6

Physical Properties

Property code	Value	Unit	Source
gf	-259.01	kJ/mol	Joback Method
hf	-480.56	kJ/mol	Joback Method
hfus	28.96	kJ/mol	Joback Method
hvap	79.46	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.508		Crippen Method
mcvol	180.850	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1902.00		NIST Webbook
rinpol	1902.00		NIST Webbook
tb	747.40	K	Joback Method
tc	952.52	K	Joback Method
tf	442.40	K	Joback Method
vc	0.686	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.99	J/mol×K	747.40	Joback Method
cpg	501.02	J/mol×K	781.59	Joback Method
cpg	511.31	J/mol×K	815.77	Joback Method
cpg	520.87	J/mol×K	849.96	Joback Method
cpg	529.73	J/mol×K	884.14	Joback Method
cpg	537.91	J/mol×K	918.33	Joback Method
cpg	545.44	J/mol×K	952.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C113793376&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

Legend

cpg:	Ideal gas heat capacity
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