2-((Prop-2-ynyloxy)carbonyl)benzoic acid

Inchi: InChI=1S/C11H8O4/c1-2-7-15-11(14)9-6-4-3-5-8(9)10(12)13/h1,3-6H,7H2,(H,12,13)
InchiKey: BEWCAUPONZLPFD-UHFFFAOYSA-N
Formula: C11H8O4
SMILES: C#CCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 204.18
CAS: 6139-61-3

Physical Properties

Property code	Value	Unit	Source
gf	-132.07	kJ/mol	Joback Method
hf	-263.02	kJ/mol	Joback Method
hfus	29.35	kJ/mol	Joback Method
hvap	75.46	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.175		Crippen Method
mcvol	148.370	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
rinpol	1731.00		NIST Webbook
rinpol	1731.00		NIST Webbook
tb	695.20	K	Joback Method
tc	910.39	K	Joback Method
tf	482.55	K	Joback Method
vc	0.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.99	J/mol×K	695.20	Joback Method
cpg	374.04	J/mol×K	731.06	Joback Method
cpg	382.44	J/mol×K	766.93	Joback Method
cpg	390.23	J/mol×K	802.79	Joback Method
cpg	397.40	J/mol×K	838.66	Joback Method
cpg	404.00	J/mol×K	874.52	Joback Method
cpg	410.03	J/mol×K	910.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6139613&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