(E)-2-((But-2-enyloxy)carbonyl)benzoic acid

Inchi: InChI=1S/C12H12O4/c1-2-3-8-16-12(15)10-7-5-4-6-9(10)11(13)14/h2-7H,8H2,1H3,(H,13
InchiKey: WCNXRKONLHFUTJ-NSCUHMNNSA-N
Formula: C12H12O4
SMILES: CC=CCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 220.22
CAS: 855233-54-4

Physical Properties

Property code	Value	Unit	Source
gf	-266.50	kJ/mol	Joback Method
hf	-458.34	kJ/mol	Joback Method
hfus	29.16	kJ/mol	Joback Method
hvap	77.78	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.118		Crippen Method
mcvol	166.760	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1835.00		NIST Webbook
tb	732.12	K	Joback Method
tc	940.27	K	Joback Method
tf	441.77	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.18	J/mol×K	732.12	Joback Method
cpg	448.54	J/mol×K	766.81	Joback Method
cpg	458.21	J/mol×K	801.50	Joback Method
cpg	467.20	J/mol×K	836.20	Joback Method
cpg	475.55	J/mol×K	870.89	Joback Method
cpg	483.29	J/mol×K	905.58	Joback Method
cpg	490.44	J/mol×K	940.27	Joback Method
dvisc	0.0010213	Pa×s	441.77	Joback Method

dvisc	0.0004435	Pa×s	490.16	Joback Method
dvisc	0.0002237	Pa×s	538.55	Joback Method
dvisc	0.0001263	Pa×s	586.95	Joback Method
dvisc	0.0000778	Pa×s	635.34	Joback Method
dvisc	0.0000513	Pa×s	683.73	Joback Method
dvisc	0.0000358	Pa×s	732.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C855233544&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
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