2-((But-3-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/h2,4-7H,1,3,8H2,(H,1
InchiKey: ITFNEGUSSAPBNU-UHFFFAOYSA-N
Formula: C12H12O4
SMILES: C=CCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 220.22
CAS: 113793-34-3

Physical Properties

Property code	Value	Unit	Source
gf	-258.88	kJ/mol	Joback Method
hf	-450.13	kJ/mol	Joback Method
hfus	27.68	kJ/mol	Joback Method
hvap	77.16	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.118		Crippen Method
mcvol	166.760	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1800.00		NIST Webbook
tb	724.64	K	Joback Method
tc	929.19	K	Joback Method
tf	445.09	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.60	J/mol×K	724.64	Joback Method
cpg	448.97	J/mol×K	758.73	Joback Method
cpg	458.64	J/mol×K	792.82	Joback Method
cpg	467.63	J/mol×K	826.91	Joback Method
cpg	475.97	J/mol×K	861.00	Joback Method
cpg	483.66	J/mol×K	895.09	Joback Method
cpg	490.74	J/mol×K	929.19	Joback Method
dvisc	0.0010920	Pa×s	445.09	Joback Method

dvisc	0.0004977	Pa×s	491.68	Joback Method
dvisc	0.0002598	Pa×s	538.27	Joback Method
dvisc	0.0001505	Pa×s	584.87	Joback Method
dvisc	0.0000944	Pa×s	631.46	Joback Method
dvisc	0.0000632	Pa×s	678.05	Joback Method
dvisc	0.0000445	Pa×s	724.64	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C113793343&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