2-((2-Methoxyethoxy)carbonyl)benzoic acid

Inchi: InChI=1S/C11H12O5/c1-15-6-7-16-11(14)9-5-3-2-4-8(9)10(12)13/h2-5H,6-7H2,1H3,(H,1
InchiKey: NGFWAKGWMSOVMP-UHFFFAOYSA-N
Formula: C11H12O5
SMILES: COCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 224.21
CAS: 16501-01-2

Physical Properties

Property code	Value	Unit	Source
gf	-460.14	kJ/mol	Joback Method
hf	-687.14	kJ/mol	Joback Method
hfus	27.56	kJ/mol	Joback Method
hvap	78.01	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	1.188		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
rinpol	1832.00		NIST Webbook
tb	727.50	K	Joback Method
tc	929.84	K	Joback Method
tf	457.81	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.65	J/mol×K	727.50	Joback Method
cpg	480.15	J/mol×K	896.11	Joback Method
cpg	472.63	J/mol×K	862.39	Joback Method
cpg	464.42	J/mol×K	828.67	Joback Method
cpg	455.52	J/mol×K	794.95	Joback Method
cpg	445.93	J/mol×K	761.22	Joback Method
cpg	486.97	J/mol×K	929.84	Joback Method
dvisc	0.0000365	Pa×s	727.50	Joback Method

dvisc	0.0000515	Pa×s	682.55	Joback Method
dvisc	0.0000761	Pa×s	637.60	Joback Method
dvisc	0.0001193	Pa×s	592.65	Joback Method
dvisc	0.0002015	Pa×s	547.71	Joback Method
dvisc	0.0003738	Pa×s	502.76	Joback Method
dvisc	0.0007826	Pa×s	457.81	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=C16501012&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