2-((2-Butoxyethoxy)carbonyl)benzoic acid

Inchi: InChI=1S/C14H18O5/c1-2-3-8-18-9-10-19-14(17)12-7-5-4-6-11(12)13(15)16/h4-7H,2-3,8
InchiKey: FYEDNKVJQMKJTP-UHFFFAOYSA-N
Formula: C14H18O5
SMILES: CCCCOCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 266.29
CAS: 21415-07-6

Physical Properties

Property code	Value	Unit	Source
gf	-434.88	kJ/mol	Joback Method
hf	-749.06	kJ/mol	Joback Method
hfus	35.33	kJ/mol	Joback Method
hvap	84.69	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.358		Crippen Method
mcvol	205.110	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	2119.00		NIST Webbook
rinpol	2119.00		NIST Webbook
tb	796.14	K	Joback Method
tc	994.91	K	Joback Method
tf	491.62	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.60	J/mol×K	796.14	Joback Method
cpg	644.98	J/mol×K	961.78	Joback Method
cpg	636.53	J/mol×K	928.65	Joback Method
cpg	627.28	J/mol×K	895.52	Joback Method
cpg	617.21	J/mol×K	862.40	Joback Method
cpg	606.32	J/mol×K	829.27	Joback Method
cpg	652.64	J/mol×K	994.91	Joback Method

dvisc	0.0000217	Pa×s	796.14	Joback Method
dvisc	0.0000308	Pa×s	745.39	Joback Method
dvisc	0.0000459	Pa×s	694.63	Joback Method
dvisc	0.0000728	Pa×s	643.88	Joback Method
dvisc	0.0001250	Pa×s	593.13	Joback Method
dvisc	0.0002374	Pa×s	542.37	Joback Method
dvisc	0.0005148	Pa×s	491.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21415076&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