2-((2-Ethoxyethoxy)carbonyl)benzoic acid

Inchi: InChI=1S/C12H14O5/c1-2-16-7-8-17-12(15)10-6-4-3-5-9(10)11(13)14/h3-6H,2,7-8H2,1H
InchiKey: FCJKZKYOELZWNI-UHFFFAOYSA-N
Formula: C12H14O5
SMILES: CCOCCOC(=O)c1ccccc1C(=O)O
Mol. weight [g/mol]: 238.24
CAS: 735274-50-7

Physical Properties

Property code	Value	Unit	Source
gf	-451.72	kJ/mol	Joback Method
hf	-707.78	kJ/mol	Joback Method
hfus	30.15	kJ/mol	Joback Method
hvap	80.23	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	1.578		Crippen Method
mcvol	176.930	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1927.00		NIST Webbook
rinpol	1927.00		NIST Webbook
tb	750.38	K	Joback Method
tc	950.99	K	Joback Method
tf	469.08	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.48	J/mol×K	750.38	Joback Method
cpg	498.30	J/mol×K	783.82	Joback Method
cpg	508.38	J/mol×K	817.25	Joback Method
cpg	517.72	J/mol×K	850.69	Joback Method
cpg	526.34	J/mol×K	884.12	Joback Method
cpg	534.22	J/mol×K	917.56	Joback Method
cpg	541.38	J/mol×K	950.99	Joback Method

dvisc	0.0006830	Pa×s	469.08	Joback Method
dvisc	0.0003222	Pa×s	515.96	Joback Method
dvisc	0.0001723	Pa×s	562.85	Joback Method
dvisc	0.0001014	Pa×s	609.73	Joback Method
dvisc	0.0000644	Pa×s	656.61	Joback Method
dvisc	0.0000434	Pa×s	703.50	Joback Method
dvisc	0.0000308	Pa×s	750.38	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=C735274507&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