

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

InChI:  
acid

InChI=1S/C13H16O6/c1-17-6-7-18-8-9-19-13(16)11-5-3-2-4-10(11)12(14)15/h2-5H,6-9H

InChIKey:

ARIYNWGPLSXJMC-UHFFFAOYSA-N

Formula:

C13H16O6

SMILES:

COCCOCCOC(=O)c1ccccc1C(=O)O

Mol. weight [g/mol]:

268.26

CAS:

207790-01-0

## Physical Properties

Property code	Value	Unit	Source
gf	-548.30	kJ/mol	Joback Method
hf	-860.64	kJ/mol	Joback Method
hfus	33.93	kJ/mol	Joback Method
hvap	84.87	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.205		Crippen Method
mvol	196.890	ml/mol	McGowan Method
pc	2543.05	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	795.68	K	Joback Method
tc	995.01	K	Joback Method
tf	502.58	K	Joback Method
vc	0.741	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.07	J/molxK	795.68	Joback Method
cpg	577.12	J/molxK	828.90	Joback Method
cpg	587.34	J/molxK	862.12	Joback Method
cpg	596.71	J/molxK	895.34	Joback Method
cpg	605.23	J/molxK	928.57	Joback Method
cpg	612.90	J/molxK	961.79	Joback Method
cpg	619.71	J/molxK	995.01	Joback Method

dvisc	0.0003797	Paxs	502.58	Joback Method
dvisc	0.0001845	Paxs	551.43	Joback Method
dvisc	0.0001008	Paxs	600.28	Joback Method
dvisc	0.0000603	Paxs	649.13	Joback Method
dvisc	0.0000388	Paxs	697.98	Joback Method
dvisc	0.0000264	Paxs	746.83	Joback Method
dvisc	0.0000189	Paxs	795.68	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C207790010&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C207790010&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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