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

Inchi: 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
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003797	Pa×s	502.58	Joback Method
dvisc	0.0001845	Pa×s	551.43	Joback Method
dvisc	0.0001008	Pa×s	600.28	Joback Method
dvisc	0.0000603	Pa×s	649.13	Joback Method
dvisc	0.0000388	Pa×s	697.98	Joback Method
dvisc	0.0000264	Pa×s	746.83	Joback Method
dvisc	0.0000189	Pa×s	795.68	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=C207790010&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