

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
mvol	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.65	J/molxK	727.50	Joback Method
cpg	445.93	J/molxK	761.22	Joback Method
cpg	455.52	J/molxK	794.95	Joback Method
cpg	464.42	J/molxK	828.67	Joback Method
cpg	472.63	J/molxK	862.39	Joback Method
cpg	480.15	J/molxK	896.11	Joback Method
cpg	486.97	J/molxK	929.84	Joback Method
dvisc	0.0007826	Paxs	457.81	Joback Method

dvisc	0.0003738	Paxs	502.76	Joback Method
dvisc	0.0002015	Paxs	547.71	Joback Method
dvisc	0.0001193	Paxs	592.65	Joback Method
dvisc	0.0000761	Paxs	637.60	Joback Method
dvisc	0.0000515	Paxs	682.55	Joback Method
dvisc	0.0000365	Paxs	727.50	Joback Method

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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

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