2-Methoxybenzoic acid, 2-methoxyethyl ester

Inchi: InChI=1S/C11H14O4/c1-13-7-8-15-11(12)9-5-3-4-6-10(9)14-2/h3-6H,7-8H2,1-2H3
InchiKey: GFYWCUFTXLOBTQ-UHFFFAOYSA-N
Formula: C11H14O4
SMILES: COCCOC(=O)c1ccccc1OC
Mol. weight [g/mol]: 210.23

Physical Properties

Property code	Value	Unit	Source
hf	-564.48	kJ/mol	Cheméo Relay (1.0)
hfus	23.06	kJ/mol	Joback Method
hvap	75.31	kJ/mol	Cheméo Relay (1.0)
ie	8.56	eV	Cheméo Relay (1.0)
log10ws	-2.04		Cheméo Relay (1.0)
logp	1.498		Crippen Method
mcvol	161.270	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1630.00		NIST Webbook
tb	572.24	K	Cheméo Relay (1.0)
tc	757.78	K	Cheméo Relay (1.0)
tf	267.43	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	395.61	J/mol×K	603.87	Joback Method
cpg	467.32	J/mol×K	809.83	Joback Method
cpg	457.16	J/mol×K	775.50	Joback Method
cpg	446.26	J/mol×K	741.17	Joback Method
cpg	434.65	J/mol×K	706.85	Joback Method
cpg	422.32	J/mol×K	672.52	Joback Method
cpg	409.31	J/mol×K	638.20	Joback Method
dvisc	0.0002766	Pa×s	486.58	Joback Method
dvisc	0.0001274	Pa×s	603.87	Joback Method
dvisc	0.0001592	Pa×s	564.77	Joback Method

dvisc	0.0002056	Pa×s	525.68	Joback Method
dvisc	0.0009817	Pa×s	369.29	Joback Method
dvisc	0.0003919	Pa×s	447.48	Joback Method
dvisc	0.0005935	Pa×s	408.39	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C948839905&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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