Benzeneacetic acid, 2-methoxy-, methyl ester

Other names:	Acetic acid, (o-methoxyphenyl)-, methyl ester
	Methyl (2-methoxyphenyl)acetate
	Methyl o-methoxyphenylacetate
	Methyl ester of o-methoxyphenylacetic acid
	2-Hydroxyphenylacetic acid, methyl ether, methyl ester
	Acetic acid, 2-methoxyphenoxy, methyl ester
Inchi:	InChI=1S/C10H12O3/c1-12-9-6-4-3-5-8(9)7-10(11)13-2/h3-6H,7H2,1-2H3
InchiKey:	BNQRSYFOIRGRKV-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COC(=O)Cc1ccccc1OC
Mol. weight [g/mol]:	180.20
CAS:	27798-60-3

Physical Properties

Property code	Value	Unit	Source
gf	-202.82	kJ/mol	Joback Method
hf	-401.69	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	52.36	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.411		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	2976.29	kPa	Joback Method
rinpol	1389.40		NIST Webbook
ripol	2024.00		NIST Webbook
ripol	2024.00		NIST Webbook
tb	558.57	K	Joback Method
tc	770.06	K	Joback Method
tf	335.79	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	323.98	J/mol×K	558.57	Joback Method
cpg	337.02	J/mol×K	593.82	Joback Method
cpg	349.42	J/mol×K	629.07	Joback Method
cpg	361.16	J/mol×K	664.31	Joback Method
cpg	372.24	J/mol×K	699.56	Joback Method
cpg	382.66	J/mol×K	734.81	Joback Method
cpg	392.43	J/mol×K	770.06	Joback Method
dvisc	0.0013400	Pa×s	335.79	Joback Method
dvisc	0.0008036	Pa×s	372.92	Joback Method
dvisc	0.0005287	Pa×s	410.05	Joback Method
dvisc	0.0003728	Pa×s	447.18	Joback Method
dvisc	0.0002774	Pa×s	484.31	Joback Method
dvisc	0.0002153	Pa×s	521.44	Joback Method
dvisc	0.0001728	Pa×s	558.57	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27798603&Units=SI
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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume