Benzeneacetic acid, 4-methoxy-, methyl ester

Other names:	Acetic acid, (p-methoxyphenyl)-, methyl ester
	(4-Methoxyphenyl)acetic acid methyl ester
	Methyl (p-methoxyphenyl)acetate
	Methyl (4-methoxyphenyl)acetate
	Methyl 2-(p-methoxyphenyl)acetate
	Phenylacetic acid, 4-methoxy, methyl ester
	Acetic acid, 4-methoxyphenoxy, methyl ester
Inchi:	InChI=1S/C10H12O3/c1-12-9-5-3-8(4-6-9)7-10(11)13-2/h3-6H,7H2,1-2H3
InchiKey:	ZQYLDVNTWDEAJI-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COC(=O)Cc1ccc(OC)cc1
Mol. weight [g/mol]:	180.20
CAS:	23786-14-3

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	1440.20		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1395.20		NIST Webbook
rinpol	1440.20		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1385.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1364.00		NIST Webbook
rinpol	1385.00		NIST Webbook
tb	537.20	K	NIST Webbook
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	382.66	J/mol×K	734.81	Joback Method
cpg	372.24	J/mol×K	699.56	Joback Method
cpg	361.16	J/mol×K	664.31	Joback Method
cpg	349.42	J/mol×K	629.07	Joback Method
cpg	337.02	J/mol×K	593.82	Joback Method
cpg	392.43	J/mol×K	770.06	Joback Method
dvisc	0.0001728	Pa×s	558.57	Joback Method
dvisc	0.0002153	Pa×s	521.44	Joback Method
dvisc	0.0002774	Pa×s	484.31	Joback Method
dvisc	0.0003728	Pa×s	447.18	Joback Method
dvisc	0.0005287	Pa×s	410.05	Joback Method
dvisc	0.0008036	Pa×s	372.92	Joback Method
dvisc	0.0013400	Pa×s	335.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	431.20	K	2.50	NIST Webbook

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=C23786143&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume