Benzeneacetic acid, 3-methoxy-

Other names:	Acetic acid, (m-methoxyphenyl)-
	(m-Methoxyphenyl)acetic acid
	(3-Methoxyphenyl)acetic acid
	3-Methoxybenzeneacetic acid
Inchi:	InChI=1S/C9H10O3/c1-12-8-4-2-3-7(5-8)6-9(10)11/h2-5H,6H2,1H3,(H,10,11)
InchiKey:	LEGPZHPSIPPYIO-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COc1cccc(CC(=O)O)c1
Mol. weight [g/mol]:	166.17
CAS:	1798-09-0

Physical Properties

Property code	Value	Unit	Source
gf	-243.06	kJ/mol	Joback Method
hf	-401.06	kJ/mol	Joback Method
hfus	19.59	kJ/mol	Joback Method
hvap	64.40	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.322		Crippen Method
mcvol	127.220	ml/mol	McGowan Method
pc	3773.04	kPa	Joback Method
rinpol	1473.00		NIST Webbook
tb	605.45	K	Joback Method
tc	807.67	K	Joback Method
tf	363.11	K	Joback Method
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.01	J/mol×K	605.45	Joback Method
cpg	348.17	J/mol×K	773.97	Joback Method
cpg	340.24	J/mol×K	740.27	Joback Method
cpg	331.76	J/mol×K	706.56	Joback Method

cpg	322.74	J/mol×K	672.86	Joback Method
cpg	313.16	J/mol×K	639.15	Joback Method
cpg	355.59	J/mol×K	807.67	Joback Method
dvisc	0.0000785	Pa×s	605.45	Joback Method
dvisc	0.0001149	Pa×s	565.06	Joback Method
dvisc	0.0001784	Pa×s	524.67	Joback Method
dvisc	0.0002980	Pa×s	484.28	Joback Method
dvisc	0.0005464	Pa×s	443.89	Joback Method
dvisc	0.0011315	Pa×s	403.50	Joback Method
dvisc	0.0027550	Pa×s	363.11	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=C1798090&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

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