

Benzeneacetic acid, «alpha»-methoxy-, (.+/-.)-

Other names:	Benzeneacetic acid, «alpha»-methoxy-, (±)- Methoxy(phenyl)acetic acid MOPA Acetic acid, methoxyphenyl- NSC 5665 2-Methoxy-2-phenylacetic acid (±)-(methoxy)phenylacetic acid
Inchi:	InChI=1S/C9H10O3/c1-12-8(9(10)11)7-5-3-2-4-6-7/h2-6,8H,1H3,(H,10,11)
InchiKey:	DIWVBIXQCNRCFE-UHFFFAOYSA-N
Formula:	C9H10O3
SMILES:	COC(C(=O)O)c1ccccc1
Mol. weight [g/mol]:	166.17
CAS:	1701-77-5

Physical Properties

Property code	Value	Unit	Source
gf	-235.87	kJ/mol	Joback Method
hf	-394.87	kJ/mol	Joback Method
hfus	16.46	kJ/mol	Joback Method
hvap	63.35	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	1.459		Crippen Method
mvol	127.220	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	600.03	K	Joback Method
tc	805.31	K	Joback Method
tf	335.59	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.57	J/mol×K	600.03	Joback Method
cpg	315.18	J/mol×K	634.24	Joback Method

cpg	325.16	J/mol×K	668.46	Joback Method
cpg	334.50	J/mol×K	702.67	Joback Method
cpg	343.24	J/mol×K	736.89	Joback Method
cpg	351.39	J/mol×K	771.10	Joback Method
cpg	358.96	J/mol×K	805.31	Joback Method
dvisc	0.0059290	Paxs	335.59	Joback Method
dvisc	0.0018822	Paxs	379.66	Joback Method
dvisc	0.0007586	Paxs	423.74	Joback Method
dvisc	0.0003629	Paxs	467.81	Joback Method
dvisc	0.0001971	Paxs	511.88	Joback Method
dvisc	0.0001179	Paxs	555.96	Joback Method
dvisc	0.0000761	Paxs	600.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1701775&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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