Benzeneacetic acid, «alpha»-methoxy-, (S)-

Other names: (S)-(-)-alpha-methoxyphenylacetic 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)/t8-/m1/s1
InchiKey: DIWVBIXQCNRCFE-MRVPVSSYSA-N
Formula: C9H10O3
SMILES: COC(C(=O)O)c1ccccc1
Mol. weight [g/mol]: 166.17
CAS: 26164-26-1

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
mcvol	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	m3/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	Pa×s	335.59	Joback Method

dvisc	0.0018822	Pa×s	379.66	Joback Method
dvisc	0.0007586	Pa×s	423.74	Joback Method
dvisc	0.0003629	Pa×s	467.81	Joback Method
dvisc	0.0001971	Pa×s	511.88	Joback Method
dvisc	0.0001179	Pa×s	555.96	Joback Method
dvisc	0.0000761	Pa×s	600.03	Joback Method

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=C26164261&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume