

(R)-(-)-«alpha»-Methoxyphenylacetic acid

Other names:	(+)-2-methoxy-2-phenylacetic acid (R)-(-)-alpha-methoxyphenylacetic acid (S)-.alpha.-methoxybenzeneacetic acid (S)-2-methoxy-2-phenylacetic acid Benzeneacetic acid, «alpha»-methoxy-, (R)-
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-/m0/s1
InchiKey:	DIWVBIXQCNRCFE-QMMMGPBSA-N
Formula:	C9H10O3
SMILES:	COC(C(=O)O)c1ccccc1
Mol. weight [g/mol]:	166.17
CAS:	3966-32-3

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/molxK	600.03	Joback Method
cpg	315.18	J/molxK	634.24	Joback Method
cpg	325.16	J/molxK	668.46	Joback Method
cpg	334.50	J/molxK	702.67	Joback Method

cpg	343.24	J/molxK	736.89	Joback Method
cpg	351.39	J/molxK	771.10	Joback Method
cpg	358.96	J/molxK	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
rhos	1311.00	kg/m3	103.00	Structural, analytical and DSC references to resolution of 2-methoxy-2-phenylacetic acid with chiral 1-cyclohexylethylamines through gas-antisolvent precipitation

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3966323&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Structural, analytical and DSC references to resolution of 2-methoxy-2-phenylacetic acid with chiral 1-cyclohexylethylamines through gas-antisolvent precipitation:	https://www.doi.org/10.1016/j.tca.2016.11.017
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

rhos:	Solid Density
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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