

4-Methoxy-3-methylphenylacetic acid

Inchi:	InChI=1S/C10H12O3/c1-7-5-8(6-10(11)12)3-4-9(7)13-2/h3-5H,6H2,1-2H3,(H,11,12)
InchiKey:	GYBWDAKGSPTODN-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COc1ccc(CC(=O)O)cc1C
Mol. weight [g/mol]:	180.20
CAS:	4513-73-9

Physical Properties

Property code	Value	Unit	Source
gf	-244.27	kJ/mol	Joback Method
hf	-433.17	kJ/mol	Joback Method
hfus	21.79	kJ/mol	Joback Method
hvap	67.29	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.631		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3306.75	kPa	Joback Method
tb	633.31	K	Joback Method
tc	833.65	K	Joback Method
tf	386.90	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.09	J/mol×K	633.31	Joback Method
cpg	359.86	J/mol×K	666.70	Joback Method
cpg	370.06	J/mol×K	700.09	Joback Method
cpg	379.69	J/mol×K	733.48	Joback Method
cpg	388.75	J/mol×K	766.87	Joback Method
cpg	397.25	J/mol×K	800.26	Joback Method
cpg	405.20	J/mol×K	833.65	Joback Method
dvisc	0.0017397	Pa×s	386.90	Joback Method
dvisc	0.0007730	Pa×s	427.97	Joback Method

dvisc	0.0003959	Pa×s	469.04	Joback Method
dvisc	0.0002258	Pa×s	510.10	Joback Method
dvisc	0.0001400	Pa×s	551.17	Joback Method
dvisc	0.0000928	Pa×s	592.24	Joback Method
dvisc	0.0000649	Pa×s	633.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4513739&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
mcvol:	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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