

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/molxK	633.31	Joback Method
cpg	359.86	J/molxK	666.70	Joback Method
cpg	370.06	J/molxK	700.09	Joback Method
cpg	379.69	J/molxK	733.48	Joback Method
cpg	388.75	J/molxK	766.87	Joback Method
cpg	397.25	J/molxK	800.26	Joback Method
cpg	405.20	J/molxK	833.65	Joback Method
dvisc	0.0017397	Paxs	386.90	Joback Method
dvisc	0.0007730	Paxs	427.97	Joback Method

dvisc	0.0003959	Paxs	469.04	Joback Method
dvisc	0.0002258	Paxs	510.10	Joback Method
dvisc	0.0001400	Paxs	551.17	Joback Method
dvisc	0.0000928	Paxs	592.24	Joback Method
dvisc	0.0000649	Paxs	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/ci9903071
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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