

3-(3-Methoxyphenyl)propanoic acid

Other names:	3-(3-Methoxyphenyl)propionic acid «beta»-(m-Methoxyphenyl)propionic acid Benzenepropanoic acid, 3-methoxy- 3-(m-methoxyphenyl)propionic acid
Inchi:	InChI=1S/C10H12O3/c1-13-9-4-2-3-8(7-9)5-6-10(11)12/h2-4,7H,5-6H2,1H3,(H,11,12)
InchiKey:	BJJQJLOZWBZEGA-UHFFFAOYSA-N
Formula:	C10H12O3
SMILES:	COc1cccc(CCC(=O)O)c1
Mol. weight [g/mol]:	180.20
CAS:	10516-71-9

Physical Properties

Property code	Value	Unit	Source
gf	-234.64	kJ/mol	Joback Method
hf	-421.70	kJ/mol	Joback Method
hfus	22.18	kJ/mol	Joback Method
hvap	66.63	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.712		Crippen Method
mcvol	141.310	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
tb	628.33	K	Joback Method
tc	827.77	K	Joback Method
tf	374.38	K	Joback Method
vc	0.530	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.22	J/molxK	628.33	Joback Method
cpg	398.96	J/molxK	794.53	Joback Method
cpg	390.39	J/molxK	761.29	Joback Method
cpg	381.24	J/molxK	728.05	Joback Method
cpg	371.50	J/molxK	694.81	Joback Method

cpg	361.17	J/mol×K	661.57	Joback Method
cpg	406.96	J/mol×K	827.77	Joback Method
dvisc	0.0000667	Paxs	628.33	Joback Method
dvisc	0.0000978	Paxs	586.00	Joback Method
dvisc	0.0001520	Paxs	543.68	Joback Method
dvisc	0.0002546	Paxs	501.35	Joback Method
dvisc	0.0004691	Paxs	459.03	Joback Method
dvisc	0.0009783	Paxs	416.70	Joback Method
dvisc	0.0024094	Paxs	374.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10516719&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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