

Adipic acid, 3-methoxy-

Inchi:	InChI=1S/C7H12O5/c1-12-5(4-7(10)11)2-3-6(8)9/h5H,2-4H2,1H3,(H,8,9)(H,10,11)
InchiKey:	TURPUAICQCJDTN-UHFFFAOYSA-N
Formula:	C7H12O5
SMILES:	COC(CCC(=O)O)CC(=O)O
Mol. weight [g/mol]:	176.17
CAS:	98962-99-3

Physical Properties

Property code	Value	Unit	Source
gf	-630.86	kJ/mol	Joback Method
hf	-854.93	kJ/mol	Joback Method
hfus	22.93	kJ/mol	Joback Method
hvap	80.05	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	0.341		Crippen Method
mcvol	130.240	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	673.64	K	Joback Method
tc	849.49	K	Joback Method
tf	397.38	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.57	J/molxK	673.64	Joback Method
cpg	355.61	J/molxK	702.95	Joback Method
cpg	363.24	J/molxK	732.26	Joback Method
cpg	370.48	J/molxK	761.56	Joback Method
cpg	377.32	J/molxK	790.87	Joback Method
cpg	383.77	J/molxK	820.18	Joback Method
cpg	389.83	J/molxK	849.49	Joback Method
dvisc	0.0036117	Paxs	397.38	Joback Method
dvisc	0.0009625	Paxs	443.42	Joback Method

dvisc	0.0003289	Paxs	489.47	Joback Method
dvisc	0.0001352	Paxs	535.51	Joback Method
dvisc	0.0000640	Paxs	581.55	Joback Method
dvisc	0.0000338	Paxs	627.60	Joback Method
dvisc	0.0000195	Paxs	673.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98962993&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

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

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