Hexanedioic acid, monomethyl ester

Other names:	5-Carbomethoxypentanoic acid
	6-Methoxy-6-oxohexanoic acid
	Hexanedioic acid, 1-methyl ester
	Methyl hemiadipate
	NSC 55113
	NSC 9389
	adipic acid, monomethyl ester
	methyl 5-carboxypentanoate
	methyl adipate
	methyl hydrogen adipate
	monomethyl adipate
Inchi:	InChI=1S/C7H12O4/c1-11-7(10)5-3-2-4-6(8)9/h2-5H2,1H3,(H,8,9)
InchiKey:	UOBSVARXACCLLH-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	COC(=O)CCCCC(=O)O
Mol. weight [g/mol]:	160.17
CAS:	627-91-8

Physical Properties

Property code	Value	Unit	Source
gf	-491.60	kJ/mol	Joback Method
hf	-697.42	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	63.76	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.804		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	581.90	K	Joback Method
tc	759.88	K	Joback Method
tf	351.56	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.49	J/mol×K	581.90	Joback Method
cpg	311.63	J/mol×K	611.56	Joback Method
cpg	320.38	J/mol×K	641.23	Joback Method
cpg	328.73	J/mol×K	670.89	Joback Method
cpg	336.70	J/mol×K	700.56	Joback Method
cpg	344.28	J/mol×K	730.22	Joback Method
cpg	351.47	J/mol×K	759.88	Joback Method
dvisc	0.0045769	Pa×s	351.56	Joback Method
dvisc	0.0018146	Pa×s	389.95	Joback Method
dvisc	0.0008492	Pa×s	428.34	Joback Method
dvisc	0.0004503	Pa×s	466.73	Joback Method
dvisc	0.0002630	Pa×s	505.12	Joback Method
dvisc	0.0001657	Pa×s	543.51	Joback Method
dvisc	0.0001109	Pa×s	581.90	Joback Method
hvapt	82.90	kJ/mol	478.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	435.20	K	1.30	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Liquid liquid equilibria of aqueous mixtures containing selected dibasic esters and/or methanol: https://www.doi.org/10.1016/j.fluid.2006.08.002

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C627918&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume