Hexanedioic acid, monoethyl ester

Other names:	Adipic acid monoethyl ester
	Monoethyl adipate
	Ethyl hydrogen adipate
	Hexanoic acid, monoethyl ester
	Monoethyladipic acid ester
	Monoethyl hexanedioate
Inchi:	InChI=1S/C8H14O4/c1-2-12-8(11)6-4-3-5-7(9)10/h2-6H2,1H3,(H,9,10)
InchiKey:	UZNLHJCCGYKCIL-UHFFFAOYSA-N
Formula:	C8H14O4
SMILES:	CCOC(=O)CCCCC(=O)O
Mol. weight [g/mol]:	174.19
CAS:	626-86-8

Physical Properties

Property code	Value	Unit	Source
gf	-483.18	kJ/mol	Joback Method
hf	-718.06	kJ/mol	Joback Method
hfus	24.95	kJ/mol	Joback Method
hvap	65.98	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.194		Crippen Method
mcvol	138.460	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	604.78	K	Joback Method
tc	781.41	K	Joback Method
tf	362.83	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.85	J/mol×K	604.78	Joback Method
cpg	358.84	J/mol×K	634.22	Joback Method
cpg	368.39	J/mol×K	663.66	Joback Method

cpg	377.50	J/mol×K	693.10	Joback Method
cpg	386.17	J/mol×K	722.54	Joback Method
cpg	394.42	J/mol×K	751.97	Joback Method
cpg	402.24	J/mol×K	781.41	Joback Method
dvisc	0.0039495	Pa×s	362.83	Joback Method
dvisc	0.0015479	Pa×s	403.15	Joback Method
dvisc	0.0007193	Pa×s	443.48	Joback Method
dvisc	0.0003798	Pa×s	483.80	Joback Method
dvisc	0.0002213	Pa×s	524.13	Joback Method
dvisc	0.0001392	Pa×s	564.45	Joback Method
dvisc	0.0000932	Pa×s	604.78	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	453.20	K	2.40	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626868&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
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