Ethylmalonic acid

Other names:	Propanedioic acid, ethyl- «alpha»-Carboxybutyric acid Malonic acid, ethyl- 1,1-Propanedicarboxylic acid
Inchi:	InChI=1S/C5H8O4/c1-2-3(4(6)7)5(8)9/h3H,2H2,1H3,(H,6,7)(H,8,9)
InchiKey:	UKFXDFUAPNAMPJ-UHFFFAOYSA-N
Formula:	C5H8O4
SMILES:	CCC(C(=O)O)C(=O)O
Mol. weight [g/mol]:	132.11
CAS:	601-75-2

Physical Properties

Property code	Value	Unit	Source
chs	-2172.20	kJ/mol	NIST Webbook
gf	-542.70	kJ/mol	Joback Method
hf	-849.80 ± 1.10	kJ/mol	NIST Webbook
hfs	-955.30 ± 1.00	kJ/mol	NIST Webbook
hfus	16.56	kJ/mol	Joback Method
hsub	105.50	kJ/mol	NIST Webbook
hsub	105.50 ± 0.50	kJ/mol	NIST Webbook
hsub	112.80 ± 2.20	kJ/mol	NIST Webbook
hvap	73.19	kJ/mol	Joback Method
log10ws	0.13		Crippen Method
logp	0.182		Crippen Method
mcvol	96.190	ml/mol	McGowan Method
pc	5251.00	kPa	Joback Method
tb	605.46	K	Joback Method
tc	783.09	K	Joback Method
tf	384.00 ± 3.00	K	NIST Webbook
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	232.92	J/mol×K	605.46	Joback Method
cpg	261.32	J/mol×K	753.49	Joback Method
cpg	256.24	J/mol×K	723.88	Joback Method
cpg	250.87	J/mol×K	694.28	Joback Method
cpg	245.20	J/mol×K	664.67	Joback Method
cpg	239.21	J/mol×K	635.07	Joback Method
cpg	266.11	J/mol×K	783.09	Joback Method
dvisc	0.0000446	Pa×s	605.46	Joback Method
dvisc	0.0000803	Pa×s	563.32	Joback Method
dvisc	0.0001588	Pa×s	521.18	Joback Method
dvisc	0.0003540	Pa×s	479.04	Joback Method
dvisc	0.0009213	Pa×s	436.89	Joback Method
dvisc	0.0029414	Pa×s	394.75	Joback Method
dvisc	0.0123933	Pa×s	352.61	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C601752&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation 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