diethyl hydroxybutanedioate

Other names:	Butanedioic acid, hydroxy-, diethyl ester, (±)- diethyl malate Malic acid, diethyl ester
Inchi:	InChI=1S/C8H14O5/c1-3-12-7(10)5-6(9)8(11)13-4-2/h6,9H,3-5H2,1-2H3
InchiKey:	VKNUORWMCINMRB-UHFFFAOYSA-N
Formula:	C8H14O5
SMILES:	CCOC(=O)CC(O)C(=O)OCC
Mol. weight [g/mol]:	190.19
CAS:	7554-12-3

Physical Properties

Property code	Value	Unit	Source
gf	-590.62	kJ/mol	Joback Method
hf	-855.56	kJ/mol	Joback Method
hfus	22.62	kJ/mol	Joback Method
hvap	68.00	kJ/mol	Joback Method
log10ws	-0.27		Crippen Method
logp	-0.136		Crippen Method
mcvol	144.330	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	1270.60		NIST Webbook
rinpol	1270.60		NIST Webbook
ripol	2060.00		NIST Webbook
ripol	2060.00		NIST Webbook
tb	626.76	K	Joback Method
tc	805.81	K	Joback Method
tf	370.06	K	Joback Method
vc	0.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.12	J/mol×K	805.81	Joback Method
cpg	373.00	J/mol×K	626.76	Joback Method

cpg	383.17	J/mol×K	656.60	Joback Method
cpg	392.88	J/mol×K	686.44	Joback Method
cpg	402.14	J/mol×K	716.29	Joback Method
cpg	410.94	J/mol×K	746.13	Joback Method
cpg	419.27	J/mol×K	775.97	Joback Method
dvisc	0.0000641	Pa×s	626.76	Joback Method
dvisc	0.0032891	Pa×s	370.06	Joback Method
dvisc	0.0012145	Pa×s	412.84	Joback Method
dvisc	0.0005407	Pa×s	455.63	Joback Method
dvisc	0.0002766	Pa×s	498.41	Joback Method
dvisc	0.0001573	Pa×s	541.19	Joback Method
dvisc	0.0000972	Pa×s	583.98	Joback Method
hvapt	59.60	kJ/mol	440.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7554123&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

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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

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