Butanedioic acid, hydroxy-, diethyl ester, (.+/-.)-

Other names: Diethyl dl-malate
Ethyl dl-malate
Butanedioic acid, hydroxy-, diethyl ester, (±)-
Diethyl hydroxybutanoate
Diethyl malate
diethyl (±)-malate

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: 626-11-9

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	1244.00		NIST Webbook
rinpol	1244.00		NIST Webbook
ripol	2062.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2058.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2048.00		NIST Webbook
ripol	2065.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2059.00		NIST Webbook
ripol	2064.00		NIST Webbook
ripol	2053.00		NIST Webbook
ripol	2039.00		NIST Webbook
ripol	2045.00		NIST Webbook

ripol	2064.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2041.00		NIST Webbook
ripol	2053.00		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	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
cpg	427.12	J/mol×K	805.81	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
dvisc	0.0000641	Pa×s	626.76	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C626119&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
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