2-Butenedioic acid (Z)-, monobutyl ester

Other names:	Maleic acid, monobutyl ester
	Butyl hydrogen maleate
	Hydrogen butyl maleate
	Monobutyl maleate
Inchi:	InChI=1S/C8H12O4/c1-2-3-6-12-8(11)5-4-7(9)10/h4-5H,2-3,6H2,1H3,(H,9,10)/b5-4-
InchiKey:	UTOVMEACOLCUCK-PLNGDYQASA-N
Formula:	C8H12O4
SMILES:	CCCCOC(=O)C=CC(=O)O
Mol. weight [g/mol]:	172.18
CAS:	925-21-3

Physical Properties

Property code	Value	Unit	Source
gf	-402.96	kJ/mol	Joback Method
hf	-600.84	kJ/mol	Joback Method
hfus	25.15	kJ/mol	Joback Method
hvap	65.94	kJ/mol	Joback Method
log10ws	-0.99		Crippen Method
logp	0.970		Crippen Method
mcvol	134.160	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
tb	608.94	K	Joback Method
tc	792.02	K	Joback Method
tf	357.75	K	Joback Method
vc	0.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.92	J/mol×K	608.94	Joback Method
cpg	370.38	J/mol×K	761.51	Joback Method
cpg	362.76	J/mol×K	730.99	Joback Method
cpg	354.71	J/mol×K	700.48	Joback Method
cpg	346.23	J/mol×K	669.97	Joback Method

cpg	337.30	J/mol×K	639.45	Joback Method
cpg	377.59	J/mol×K	792.02	Joback Method
dvisc	0.0000782	Pa×s	608.94	Joback Method
dvisc	0.0001178	Pa×s	567.08	Joback Method
dvisc	0.0001893	Pa×s	525.21	Joback Method
dvisc	0.0003302	Pa×s	483.35	Joback Method
dvisc	0.0006401	Pa×s	441.48	Joback Method
dvisc	0.0014254	Pa×s	399.62	Joback Method
dvisc	0.0038287	Pa×s	357.75	Joback Method

Sources

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=C925213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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