Butanoic acid, 2,3-dihydroxy-2-methyl, erythro, methyl ester

Inchi: InChI=1S/C6H12O4/c1-4(7)6(2,9)5(8)10-3/h4,7,9H,1-3H3/t4-,6-/m0/s1

InchiKey: XKXDXWAQHUEJGN-NJGYIYPDSA-N

Formula: C6H12O4

SMILES: COC(=O)C(C)(O)C(C)O

Mol. weight [g/mol]: 148.16

Physical Properties

Property code	Value	Unit	Source
gf	-507.52	kJ/mol	Joback Method
hf	-730.46	kJ/mol	Joback Method
hfus	11.32	kJ/mol	Joback Method
hvap	69.78	kJ/mol	Joback Method
log10ws	0.05		Crippen Method
logp	-0.709		Crippen Method
mcvol	114.580	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
rinpol	973.00		NIST Webbook
tb	593.66	K	Joback Method
tc	770.02	K	Joback Method
tf	338.60	K	Joback Method
vc	0.416	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.05	J/mol×K	593.66	Joback Method
cpg	331.40	J/mol×K	740.63	Joback Method
cpg	324.73	J/mol×K	711.23	Joback Method
cpg	317.67	J/mol×K	681.84	Joback Method
cpg	310.21	J/mol×K	652.45	Joback Method
cpg	302.34	J/mol×K	623.05	Joback Method
cpg	337.71	J/mol×K	770.02	Joback Method
dvisc	0.0000317	Pa×s	593.66	Joback Method
dvisc	0.0000604	Pa×s	551.15	Joback Method

dvisc	0.0001281	Pa×s	508.64	Joback Method
dvisc	0.0003118	Pa×s	466.13	Joback Method
dvisc	0.0009071	Pa×s	423.62	Joback Method
dvisc	0.0033496	Pa×s	381.11	Joback Method
dvisc	0.0171705	Pa×s	338.60	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=R395250&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume