

Butanoic acid, 2,3-dihydroxy-2-methyl, threo, 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-UJURSFKZSA-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	968.00		NIST Webbook
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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/molxK	593.66	Joback Method
cpg	302.34	J/molxK	623.05	Joback Method
cpg	310.21	J/molxK	652.45	Joback Method
cpg	317.67	J/molxK	681.84	Joback Method
cpg	324.73	J/molxK	711.23	Joback Method
cpg	331.40	J/molxK	740.63	Joback Method
cpg	337.71	J/molxK	770.02	Joback Method
dvisc	0.0171705	Paxs	338.60	Joback Method

dvisc	0.0033496	Paxs	381.11	Joback Method
dvisc	0.0009071	Paxs	423.62	Joback Method
dvisc	0.0003118	Paxs	466.13	Joback Method
dvisc	0.0001281	Paxs	508.64	Joback Method
dvisc	0.0000604	Paxs	551.15	Joback Method
dvisc	0.0000317	Paxs	593.66	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R395265&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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