(R)-3-Hydroxybutyric acid, methyl ether, methyl ester

Other names: Methyl (3R)-3-methoxybutanoate
Inchi: InChI=1S/C6H12O3/c1-5(8-2)4-6(7)9-3/h5H,4H2,1-3H3
InchiKey: NRMQYDNCUDPVAI-UHFFFAOYSA-N
Formula: C6H12O3
SMILES: COC(=O)CC(C)OC
Mol. weight [g/mol]: 132.16

Physical Properties

Property code	Value	Unit	Source
gf	-341.72	kJ/mol	Joback Method
hf	-549.47	kJ/mol	Joback Method
hfus	11.75	kJ/mol	Joback Method
hvap	40.13	kJ/mol	Joback Method
log10ws	-0.40		Crippen Method
logp	0.584		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	891.40		NIST Webbook
rinpol	886.00		NIST Webbook
rinpol	892.60		NIST Webbook
rinpol	892.60		NIST Webbook
rinpol	886.00		NIST Webbook
tb	434.95	K	Joback Method
tc	616.32	K	Joback Method
tf	236.77	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.96	J/mol×K	434.95	Joback Method
cpg	269.18	J/mol×K	586.09	Joback Method
cpg	260.32	J/mol×K	555.87	Joback Method
cpg	251.15	J/mol×K	525.64	Joback Method

cpg	241.69	J/mol×K	495.41	Joback Method
cpg	231.96	J/mol×K	465.18	Joback Method
cpg	277.74	J/mol×K	616.32	Joback Method
dvisc	0.0002290	Pa×s	434.95	Joback Method
dvisc	0.0002985	Pa×s	401.92	Joback Method
dvisc	0.0004081	Pa×s	368.89	Joback Method
dvisc	0.0005932	Pa×s	335.86	Joback Method
dvisc	0.0009358	Pa×s	302.83	Joback Method
dvisc	0.0016505	Pa×s	269.80	Joback Method
dvisc	0.0034104	Pa×s	236.77	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U332956&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

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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