Butanoic acid, 4-methoxy-, methyl ester

Other names:	Butyric acid, 4-methoxy-, methyl ester
	Methyl 4-methoxybutyrate
	Methyl 4-methoxybutanoate
Inchi:	InChI=1S/C6H12O3/c1-8-5-3-4-6(7)9-2/h3-5H2,1-2H3
InchiKey:	VHDGWXQBVWAMJA-UHFFFAOYSA-N
Formula:	C6H12O3
SMILES:	COCCCC(=O)OC
Mol. weight [g/mol]:	132.16
CAS:	29006-01-7

Physical Properties

Property code	Value	Unit	Source
gf	-339.28	kJ/mol	Joback Method
hf	-544.19	kJ/mol	Joback Method
hfus	15.27	kJ/mol	Joback Method
hvap	40.52	kJ/mol	Joback Method
log10ws	-0.28		Crippen Method
logp	0.586		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	435.39	K	Joback Method
tc	612.77	K	Joback Method
tf	251.77	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.86	J/mol×K	435.39	Joback Method
cpg	231.56	J/mol×K	464.95	Joback Method
cpg	241.01	J/mol×K	494.52	Joback Method
cpg	250.20	J/mol×K	524.08	Joback Method
cpg	259.12	J/mol×K	553.64	Joback Method
cpg	267.77	J/mol×K	583.20	Joback Method

cpg	276.12	J/mol×K	612.77	Joback Method
dvisc	0.0023571	Pa×s	251.77	Joback Method
dvisc	0.0013093	Pa×s	282.37	Joback Method
dvisc	0.0008159	Pa×s	312.98	Joback Method
dvisc	0.0005532	Pa×s	343.58	Joback Method
dvisc	0.0003996	Pa×s	374.18	Joback Method
dvisc	0.0003033	Pa×s	404.79	Joback Method
dvisc	0.0002392	Pa×s	435.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29006017&Units=SI

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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