

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	m ³ /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	Paxs	251.77	Joback Method
dvisc	0.0013093	Paxs	282.37	Joback Method
dvisc	0.0008159	Paxs	312.98	Joback Method
dvisc	0.0005532	Paxs	343.58	Joback Method
dvisc	0.0003996	Paxs	374.18	Joback Method
dvisc	0.0003033	Paxs	404.79	Joback Method
dvisc	0.0002392	Paxs	435.39	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=C29006017&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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