3-Methoxybutanal

Inchi: InChI=1S/C5H10O2/c1-5(7-2)3-4-6/h4-5H,3H2,1-2H3
InchiKey: VVXNMKJDQVBOLT-UHFFFAOYSA-N
Formula: C5H10O2
SMILES: COC(C)CC=O
Mol. weight [g/mol]: 102.13
CAS: 5281-76-5

Physical Properties

Property code	Value	Unit	Source
gf	-215.74	kJ/mol	Joback Method
hf	-369.61	kJ/mol	Joback Method
hfus	8.66	kJ/mol	Joback Method
hvap	35.47	kJ/mol	Joback Method
log10ws	-0.39		Crippen Method
logp	0.610		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	716.00		NIST Webbook
rinpol	724.00		NIST Webbook
rinpol	716.00		NIST Webbook
tb	384.44	K	Joback Method
tc	561.97	K	Joback Method
tf	195.34	K	Joback Method
vc	0.344	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	165.58	J/mol×K	384.44	Joback Method
cpg	205.22	J/mol×K	532.38	Joback Method
cpg	197.81	J/mol×K	502.79	Joback Method
cpg	190.13	J/mol×K	473.21	Joback Method
cpg	182.20	J/mol×K	443.62	Joback Method
cpg	174.02	J/mol×K	414.03	Joback Method

cpg	212.38	J/mol×K	561.97	Joback Method
dvisc	0.0002815	Pa×s	384.44	Joback Method
dvisc	0.0003663	Pa×s	352.92	Joback Method
dvisc	0.0005019	Pa×s	321.41	Joback Method
dvisc	0.0007365	Pa×s	289.89	Joback Method
dvisc	0.0011867	Pa×s	258.37	Joback Method
dvisc	0.0021832	Pa×s	226.86	Joback Method
dvisc	0.0048899	Pa×s	195.34	Joback Method

Sources

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=C5281765&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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