

Propanal, 3-methoxy-

Inchi:	InChI=1S/C4H8O2/c1-6-4-2-3-5/h3H,2,4H2,1H3
InchiKey:	OXGJKCALURPRCN-UHFFFAOYSA-N
Formula:	C4H8O2
SMILES:	COCCC=O
Mol. weight [g/mol]:	88.11
CAS:	2806-84-0

Physical Properties

Property code	Value	Unit	Source
gf	-221.72	kJ/mol	Joback Method
hf	-343.69	kJ/mol	Joback Method
hfus	9.59	kJ/mol	Joback Method
hvap	33.63	kJ/mol	Joback Method
log10ws	0.14		Crippen Method
logp	0.222		Crippen Method
mcvol	74.660	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	362.00	K	Joback Method
tc	535.90	K	Joback Method
tf	199.07	K	Joback Method
vc	0.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	132.08	J/mol×K	362.00	Joback Method
cpg	163.60	J/mol×K	506.91	Joback Method
cpg	157.65	J/mol×K	477.93	Joback Method
cpg	151.51	J/mol×K	448.95	Joback Method
cpg	145.20	J/mol×K	419.97	Joback Method
cpg	138.73	J/mol×K	390.98	Joback Method
cpg	169.38	J/mol×K	535.90	Joback Method
dvisc	0.0002824	Pa×s	362.00	Joback Method
dvisc	0.0003535	Pa×s	334.85	Joback Method

dvisc	0.0004603	Pa×s	307.69	Joback Method
dvisc	0.0006309	Pa×s	280.53	Joback Method
dvisc	0.0009250	Pa×s	253.38	Joback Method
dvisc	0.0014868	Pa×s	226.22	Joback Method
dvisc	0.0027202	Pa×s	199.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2806840&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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