

trans-4-Methoxy-3-buten-2-one

Other names:	(E)-4-methoxy-3-buten-2-one
Inchi:	InChI=1S/C5H8O2/c1-5(6)3-4-7-2/h3-4H,1-2H3/b4-3+
InchiKey:	VLLHEPHWWIDUSS-ONEGZZNKSA-N
Formula:	C5H8O2
SMILES:	COC=CC(C)=O
Mol. weight [g/mol]:	100.12
CAS:	51731-17-0

Physical Properties

Property code	Value	Unit	Source
gf	-162.48	kJ/mol	Joback Method
hf	-274.11	kJ/mol	Joback Method
hfus	11.69	kJ/mol	Joback Method
hvap	35.84	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.735		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	473.20	K	NIST Webbook
tc	582.22	K	Joback Method
tf	213.19	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.24	J/mol×K	394.25	Joback Method
cpg	156.32	J/mol×K	425.58	Joback Method
cpg	164.08	J/mol×K	456.91	Joback Method
cpg	171.53	J/mol×K	488.23	Joback Method
cpg	178.67	J/mol×K	519.56	Joback Method
cpg	185.52	J/mol×K	550.89	Joback Method
cpg	192.07	J/mol×K	582.22	Joback Method
dvisc	0.0025463	Pa×s	213.19	Joback Method

dvisc	0.0013230	Pa×s	243.37	Joback Method
dvisc	0.0007942	Pa×s	273.54	Joback Method
dvisc	0.0005276	Pa×s	303.72	Joback Method
dvisc	0.0003774	Pa×s	333.90	Joback Method
dvisc	0.0002854	Pa×s	364.07	Joback Method
dvisc	0.0002253	Pa×s	394.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51731170&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/88-057-2/trans-4-Methoxy-3-buten-2-one.pdf>

Generated by Cheméo on 2025-12-22 22:11:18.344440779 +0000 UTC m=+6189675.874481433.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.