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
InchiKey: VLLHEPHWWIDUSS-ONEGZZNKSA-N
Formula: C5H8O2
SMILES: CO/C=C/C(C)=O
Mol. weight [g/mol]: 100.12

Physical Properties

Property code	Value	Unit	Source
hf	-314.77	kJ/mol	Cheméo Relay (1.0)
hfus	11.69	kJ/mol	Joback Method
ie	8.87	eV	Cheméo Relay (1.0)
logp	0.735		Crippen Method
mcvol	84.450	ml/mol	McGowan Method
tb	473.20	K	NIST Webbook
tf	273.36	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51731170&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point