4-METHOXY-2-BUTANONE

Inchi: InChI=1S/C5H10O2/c1-5(6)3-4-7-2/h3-4H2,1-2H3
InchiKey: DRWOJIIXBYNGGW-UHFFFAOYSA-N
Formula: C5H10O2
SMILES: COCCC(C)=O
Mol. weight [g/mol]: 102.13

Physical Properties

Property code	Value	Unit	Source
af	0.4054		Cheméo Relay (1.0)
gf	-242.70	kJ/mol	Joback Method
hf	-375.20	kJ/mol	Cheméo Relay (1.0)
hfus	11.49	kJ/mol	Joback Method
hvap	43.18	kJ/mol	Cheméo Relay (1.0)
ie	9.37	eV	NIST Webbook
log10ws	0.94		Cheméo Relay (1.0)
logp	0.612		Crippen Method
mcvol	88.750	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
tb	413.53	K	Cheméo Relay (1.0)
tc	581.93	K	Cheméo Relay (1.0)
tf	209.32	K	Cheméo Relay (1.0)
vc	0.315	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.46	J/mol×K	390.09	Joback Method
cpg	210.46	J/mol×K	568.66	Joback Method
cpg	203.26	J/mol×K	538.90	Joback Method
cpg	195.80	J/mol×K	509.14	Joback Method
cpg	188.08	J/mol×K	479.38	Joback Method
cpg	180.12	J/mol×K	449.61	Joback Method
cpg	171.91	J/mol×K	419.85	Joback Method
dvisc	0.0006307	Pa×s	304.18	Joback Method

dvisc	0.0002744	Pa×s	390.09	Joback Method
dvisc	0.0003466	Pa×s	361.45	Joback Method
dvisc	0.0004556	Pa×s	332.82	Joback Method
dvisc	0.0027914	Pa×s	218.27	Joback Method
dvisc	0.0009341	Pa×s	275.54	Joback Method
dvisc	0.0015155	Pa×s	246.91	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6975855&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

af: Acentric Factor
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
ie: Ionization energy
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