CH2COCH3

Other names: CH2COCH3
Inchi: InChI=1S/C3H5O/c1-3(2)4/h1H2,2H3
InchiKey: HNUKTDKISXPDPA-UHFFFAOYSA-N
Formula: C3H5O
SMILES: [CH2]C(C)=O
Mol. weight [g/mol]: 57.07

Physical Properties

Property code	Value	Unit	Source
af	0.3500		Cheméo Relay (1.0)
gf	-102.16	kJ/mol	Joback Method
hf	-136.42	kJ/mol	Cheméo Relay (1.0)
hfus	6.81	kJ/mol	Joback Method
hvap	26.08	kJ/mol	Cheméo Relay (1.0)
ie	9.34	eV	Cheméo Relay (1.0)
log10ws	0.49		Cheméo Relay (1.0)
logp	0.409		Crippen Method
mcvol	52.550	ml/mol	McGowan Method
pc	5109.34	kPa	Joback Method
tb	340.87	K	Cheméo Relay (1.0)
tc	492.68	K	Cheméo Relay (1.0)
tf	176.56	K	Cheméo Relay (1.0)
vc	0.198	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	74.27	J/mol×K	321.21	Joback Method
cpg	79.67	J/mol×K	350.36	Joback Method
cpg	84.75	J/mol×K	379.51	Joback Method
cpg	89.50	J/mol×K	408.65	Joback Method
cpg	93.96	J/mol×K	437.80	Joback Method
cpg	98.13	J/mol×K	466.95	Joback Method
cpg	102.05	J/mol×K	496.10	Joback Method

dvisc	0.0006124	Pa×s	189.87	Joback Method
dvisc	0.0004966	Pa×s	211.76	Joback Method
dvisc	0.0004188	Pa×s	233.65	Joback Method
dvisc	0.0003637	Pa×s	255.54	Joback Method
dvisc	0.0003229	Pa×s	277.43	Joback Method
dvisc	0.0002918	Pa×s	299.32	Joback Method
dvisc	0.0002673	Pa×s	321.21	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B1003883&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

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