Ethanone, 1-(3,4-dihydro-6-methyl-2H-pyran-2-yl)-

Other names: 2-Acetyl-6-methyl-2,3-dihydropyran
3,4-Dihydro-6-methyl-2-acetyl-2H-pyran
Ketone, 3,4-dihydro-6-methyl-2H-pyran-2-yl methyl

Inchi: InChI=1S/C8H12O2/c1-6-4-3-5-8(10-6)7(2)9/h4,8H,3,5H2,1-2H3

InchiKey: QIYRGBNUCNZLNY-UHFFFAOYSA-N

Formula: C8H12O2

SMILES: CC(=O)C1CCC=C(C)O1

Mol. weight [g/mol]: 140.18

CAS: 28450-02-4

Physical Properties

Property code	Value	Unit	Source
gf	-153.78	kJ/mol	Joback Method
hf	-352.40	kJ/mol	Joback Method
hfus	18.72	kJ/mol	Joback Method
hvap	46.04	kJ/mol	Joback Method
ie	8.62	eV	NIST Webbook
log10ws	-1.89		Crippen Method
logp	1.658		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	452.00	K	NIST Webbook
tc	702.63	K	Joback Method
tf	277.08	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.09	J/mol×K	486.95	Joback Method
cpg	267.40	J/mol×K	522.90	Joback Method
cpg	280.94	J/mol×K	558.84	Joback Method
cpg	293.74	J/mol×K	594.79	Joback Method
cpg	305.81	J/mol×K	630.73	Joback Method

cpg	317.17	J/mol×K	666.68	Joback Method
cpg	327.83	J/mol×K	702.63	Joback Method
dvisc	0.0034450	Pa×s	277.08	Joback Method
dvisc	0.0018672	Pa×s	312.06	Joback Method
dvisc	0.0011450	Pa×s	347.04	Joback Method
dvisc	0.0007680	Pa×s	382.01	Joback Method
dvisc	0.0005507	Pa×s	416.99	Joback Method
dvisc	0.0004158	Pa×s	451.97	Joback Method
dvisc	0.0003269	Pa×s	486.95	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C28450024&Units=SI

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
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