C2H5C(CH3)2COCH3

Other names: 3,3-Dimethyl-2-pentanone
3,3-Dimethylpentan-2-one
Inchi: InChI=1S/C7H14O/c1-5-7(3,4)6(2)8/h5H2,1-4H3
InchiKey: QSHJLBQLQVSEFV-UHFFFAOYSA-N
Formula: C7H14O
SMILES: CCC(C)(C)C(C)=O
Mol. weight [g/mol]: 114.19
CAS: 20669-04-9

Physical Properties

Property code	Value	Unit	Source
gf	-118.02	kJ/mol	Joback Method
hf	-303.80 ± 1.70	kJ/mol	NIST Webbook
hfus	8.07	kJ/mol	Joback Method
hvap	36.63	kJ/mol	Joback Method
ie	9.02 ± 0.01	eV	NIST Webbook
log10ws	-1.79		Crippen Method
logp	2.012		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	403.65 ± 1.00	K	NIST Webbook
tb	403.75 ± 1.00	K	NIST Webbook
tb	404.65 ± 1.00	K	NIST Webbook
tb	405.15 ± 1.00	K	NIST Webbook
tb	404.15 ± 1.00	K	NIST Webbook
tb	405.65 ± 1.00	K	NIST Webbook
tb	402.15 ± 5.00	K	NIST Webbook
tc	598.48	K	Joback Method
tf	221.00	K	Joback Method
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	217.39	J/mol×K	410.20	Joback Method
cpg	230.12	J/mol×K	441.58	Joback Method
cpg	242.19	J/mol×K	472.96	Joback Method
cpg	253.64	J/mol×K	504.34	Joback Method
cpg	264.49	J/mol×K	535.72	Joback Method
cpg	274.76	J/mol×K	567.10	Joback Method
cpg	284.48	J/mol×K	598.48	Joback Method
dvisc	0.0067880	Pa×s	221.00	Joback Method
dvisc	0.0029812	Pa×s	252.53	Joback Method
dvisc	0.0015717	Pa×s	284.07	Joback Method
dvisc	0.0009417	Pa×s	315.60	Joback Method
dvisc	0.0006193	Pa×s	347.13	Joback Method
dvisc	0.0004367	Pa×s	378.67	Joback Method
dvisc	0.0003249	Pa×s	410.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49580e+01
Coeff. B	-3.62517e+03
Coeff. C	-5.33920e+01
Temperature range (K), min.	300.50
Temperature range (K), max.	429.19

Sources

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=C20669049&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume