2,4-Pentanedione, 3-(1-methylethyl)-

Other names:	2,4-Pentanedione, 3-isopropyl-
	Isopropylacetylacetone
	3-Isopropyl-2,4-pentanedione
	3-(1-Methylethyl)pentane-2,4-dione
Inchi:	InChI=1S/C8H14O2/c1-5(2)8(6(3)9)7(4)10/h5,8H,1-4H3
InchiKey:	BPIHCIRSGQKCLT-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CC(=O)C(C(C)=O)C(C)C
Mol. weight [g/mol]:	142.20
CAS:	1540-38-1

Physical Properties

Property code	Value	Unit	Source
gf	-246.24	kJ/mol	Joback Method
hf	-448.90	kJ/mol	NIST Webbook
hfus	12.63	kJ/mol	Joback Method
hvap	46.12	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	1.437		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	489.30	K	Joback Method
tc	683.26	K	Joback Method
tf	249.78	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.64	J/mol×K	489.30	Joback Method
cpg	288.08	J/mol×K	521.63	Joback Method
cpg	299.94	J/mol×K	553.95	Joback Method
cpg	311.23	J/mol×K	586.28	Joback Method
cpg	321.97	J/mol×K	618.61	Joback Method

cpg	332.16	J/mol×K	650.93	Joback Method
cpg	341.82	J/mol×K	683.26	Joback Method
dvisc	0.0073425	Pa×s	249.78	Joback Method
dvisc	0.0029847	Pa×s	289.70	Joback Method
dvisc	0.0015088	Pa×s	329.62	Joback Method
dvisc	0.0008839	Pa×s	369.54	Joback Method
dvisc	0.0005747	Pa×s	409.46	Joback Method
dvisc	0.0004034	Pa×s	449.38	Joback Method
dvisc	0.0002999	Pa×s	489.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1540381&Units=SI
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

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
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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.