

Acetoin acetate

Inchi:	InChI=1S/C6H10O3/c1-4(7)5(2)9-6(3)8/h5H,1-3H3
InchiKey:	ZKPTYCJWRHHBOW-UHFFFAOYSA-N
Formula:	C6H10O3
SMILES:	CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	130.14

Physical Properties

Property code	Value	Unit	Source
gf	-365.64	kJ/mol	Joback Method
hf	-529.83	kJ/mol	Joback Method
hfus	12.16	kJ/mol	Joback Method
hvap	44.46	kJ/mol	Joback Method
log10ws	-0.59		Crippen Method
logp	0.527		Crippen Method
mcvol	104.410	ml/mol	McGowan Method
pc	3555.77	kPa	Joback Method
ripol	1389.00		NIST Webbook
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tb	466.40	K	Joback Method
tc	659.46	K	Joback Method
tf	264.47	K	Joback Method
vc	0.396	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.20	J/molxK	466.40	Joback Method
cpg	224.83	J/molxK	498.58	Joback Method
cpg	234.10	J/molxK	530.75	Joback Method
cpg	243.00	J/molxK	562.93	Joback Method
cpg	251.53	J/molxK	595.11	Joback Method
cpg	259.68	J/molxK	627.28	Joback Method
cpg	267.46	J/molxK	659.46	Joback Method
dvisc	0.0036503	Paxs	264.47	Joback Method

dvisc	0.0019016	Paxs	298.12	Joback Method
dvisc	0.0011308	Paxs	331.78	Joback Method
dvisc	0.0007400	Paxs	365.44	Joback Method
dvisc	0.0005201	Paxs	399.09	Joback Method
dvisc	0.0003862	Paxs	432.75	Joback Method
dvisc	0.0002994	Paxs	466.40	Joback Method

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=R610376&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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