

Acetoin hexanoate

Inchi:	InChI=1S/C10H18O3/c1-4-5-6-7-10(12)13-9(3)8(2)11/h9H,4-7H2,1-3H3
InchiKey:	SJTOOZDKCFKYJW-UHFFFAOYSA-N
Formula:	C10H18O3
SMILES:	CCCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	186.25

Physical Properties

Property code	Value	Unit	Source
gf	-331.96	kJ/mol	Joback Method
hf	-612.39	kJ/mol	Joback Method
hfus	22.52	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.087		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1234.00		NIST Webbook
rinpol	1233.00		NIST Webbook
tb	557.92	K	Joback Method
tc	742.33	K	Joback Method
tf	309.55	K	Joback Method
vc	0.620	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.55	J/molxK	557.92	Joback Method
cpg	404.21	J/molxK	588.66	Joback Method
cpg	417.28	J/molxK	619.39	Joback Method
cpg	429.76	J/molxK	650.13	Joback Method
cpg	441.66	J/molxK	680.86	Joback Method
cpg	452.99	J/molxK	711.60	Joback Method
cpg	463.74	J/molxK	742.33	Joback Method
dvisc	0.0034308	Paxs	309.55	Joback Method

dvisc	0.0016605	Paxs	350.95	Joback Method
dvisc	0.0009367	Paxs	392.34	Joback Method
dvisc	0.0005894	Paxs	433.74	Joback Method
dvisc	0.0004021	Paxs	475.13	Joback Method
dvisc	0.0002916	Paxs	516.53	Joback Method
dvisc	0.0002218	Paxs	557.92	Joback Method

Sources

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=R66273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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