

Hexyl pyruvate

Inchi:	InChI=1S/C9H16O3/c1-3-4-5-6-7-12-9(11)8(2)10/h3-7H2,1-2H3
InchiKey:	HMSXMTIZDANRFV-UHFFFAOYSA-N
Formula:	C9H16O3
SMILES:	CCCCCOC(=O)C(C)=O
Mol. weight [g/mol]:	172.22

Physical Properties

Property code	Value	Unit	Source
gf	-337.94	kJ/mol	Joback Method
hf	-586.47	kJ/mol	Joback Method
hfus	23.45	kJ/mol	Joback Method
hvap	51.53	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.699		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
rinpol	1164.00		NIST Webbook
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tb	535.48	K	Joback Method
tc	718.27	K	Joback Method
tf	313.28	K	Joback Method
vc	0.570	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.51	J/molxK	535.48	Joback Method
cpg	356.03	J/molxK	565.94	Joback Method
cpg	368.04	J/molxK	596.41	Joback Method
cpg	379.53	J/molxK	626.87	Joback Method
cpg	390.51	J/molxK	657.34	Joback Method
cpg	400.99	J/molxK	687.80	Joback Method
cpg	410.97	J/molxK	718.27	Joback Method
dvisc	0.0026992	Paxs	313.28	Joback Method

dvisc	0.0014842	Paxs	350.31	Joback Method
dvisc	0.0009150	Paxs	387.35	Joback Method
dvisc	0.0006138	Paxs	424.38	Joback Method
dvisc	0.0004390	Paxs	461.41	Joback Method
dvisc	0.0003300	Paxs	498.45	Joback Method
dvisc	0.0002580	Paxs	535.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R11876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
log_p:	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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