

methyl 3-methyl-4-oxopentanoate

Inchi:	InChI=1S/C7H12O3/c1-5(6(2)8)4-7(9)10-3/h5H,4H2,1-3H3
InchiKey:	DPWCQWVJGUAQCY-UHFFFAOYSA-N
Formula:	C7H12O3
SMILES:	COC(=O)CC(C)C(C)=O
Mol. weight [g/mol]:	144.17

Physical Properties

Property code	Value	Unit	Source
gf	-357.22	kJ/mol	Joback Method
hf	-550.47	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	46.69	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.775		Crippen Method
mvol	118.500	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
ripol	1532.00		NIST Webbook
ripol	1532.00		NIST Webbook
tb	489.28	K	Joback Method
tc	680.12	K	Joback Method
tf	275.74	K	Joback Method
vc	0.452	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.03	J/molxK	489.28	Joback Method
cpg	266.86	J/molxK	521.09	Joback Method
cpg	277.26	J/molxK	552.89	Joback Method
cpg	287.23	J/molxK	584.70	Joback Method
cpg	296.77	J/molxK	616.51	Joback Method
cpg	305.87	J/molxK	648.32	Joback Method
cpg	314.54	J/molxK	680.12	Joback Method
dvisc	0.0036824	Paxs	275.74	Joback Method

dvisc	0.0018798	Paxs	311.33	Joback Method
dvisc	0.0011016	Paxs	346.92	Joback Method
dvisc	0.0007130	Paxs	382.51	Joback Method
dvisc	0.0004970	Paxs	418.10	Joback Method
dvisc	0.0003666	Paxs	453.69	Joback Method
dvisc	0.0002827	Paxs	489.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U143363&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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