

Succinaldehydic acid, methyl ester

Other names:	methyl 4-oxobutyrate
Inchi:	InChI=1S/C5H8O3/c1-8-5(7)3-2-4-6/h4H,2-3H2,1H3
InchiKey:	DLZVZNAPRCRXEG-UHFFFAOYSA-N
Formula:	C5H8O3
SMILES:	COC(=O)CCC=O
Mol. weight [g/mol]:	116.12
CAS:	13865-19-5

Physical Properties

Property code	Value	Unit	Source
gf	-342.22	kJ/mol	Joback Method
hf	-476.91	kJ/mol	Joback Method
hfus	13.78	kJ/mol	Joback Method
hvap	42.60	kJ/mol	Joback Method
log10ws	-0.06		Crippen Method
logp	0.138		Crippen Method
mcvol	90.320	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
tb	438.75	K	Joback Method
tc	624.44	K	Joback Method
tf	260.27	K	Joback Method
vc	0.356	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.53	J/molxK	438.75	Joback Method
cpg	186.26	J/molxK	469.70	Joback Method
cpg	193.74	J/molxK	500.65	Joback Method
cpg	200.94	J/molxK	531.59	Joback Method
cpg	207.89	J/molxK	562.54	Joback Method
cpg	214.56	J/molxK	593.49	Joback Method
cpg	220.95	J/molxK	624.44	Joback Method
dvisc	0.0028608	Paxs	260.27	Joback Method

dvisc	0.0016857	Paxs	290.02	Joback Method
dvisc	0.0010960	Paxs	319.76	Joback Method
dvisc	0.0007668	Paxs	349.51	Joback Method
dvisc	0.0005674	Paxs	379.26	Joback Method
dvisc	0.0004386	Paxs	409.00	Joback Method
dvisc	0.0003511	Paxs	438.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13865195&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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