2-Keto-octanoic acid, methyl ester

Inchi: InChI=1S/C9H16O3/c1-3-4-5-6-7-8(10)9(11)12-2/h3-7H2,1-2H3
InchiKey: JCVKROPMQGWQGA-UHFFFAOYSA-N
Formula: C9H16O3
SMILES: CCCCCCC(=O)C(=O)OC
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	1200.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1200.00		NIST Webbook
tb	535.48	K	Joback Method
tc	718.27	K	Joback Method
tf	313.28	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.51	J/mol×K	535.48	Joback Method
cpg	400.99	J/mol×K	687.80	Joback Method
cpg	390.51	J/mol×K	657.34	Joback Method
cpg	379.53	J/mol×K	626.87	Joback Method
cpg	368.04	J/mol×K	596.41	Joback Method
cpg	356.03	J/mol×K	565.94	Joback Method

cpg	410.97	J/mol×K	718.27	Joback Method
dvisc	0.0002580	Pa×s	535.48	Joback Method
dvisc	0.0003300	Pa×s	498.45	Joback Method
dvisc	0.0004390	Pa×s	461.41	Joback Method
dvisc	0.0006138	Pa×s	424.38	Joback Method
dvisc	0.0009150	Pa×s	387.35	Joback Method
dvisc	0.0014842	Pa×s	350.31	Joback Method
dvisc	0.0026992	Pa×s	313.28	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=R78&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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