methyl 5-hydroxyoctanoate

Inchi: InChI=1S/C9H18O3/c1-3-5-8(10)6-4-7-9(11)12-2/h8,10H,3-7H2,1-2H3
InchiKey: XMQPWFCBPDENRU-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: CCCC(O)CCCC(=O)OC
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
gf	-348.28	kJ/mol	Joback Method
hf	-631.40	kJ/mol	Joback Method
hfus	22.42	kJ/mol	Joback Method
hvap	61.08	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.491		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
ripol	1994.00		NIST Webbook
ripol	1994.00		NIST Webbook
tb	573.35	K	Joback Method
tc	743.84	K	Joback Method
tf	309.17	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.44	J/mol×K	573.35	Joback Method
cpg	392.26	J/mol×K	601.77	Joback Method
cpg	403.60	J/mol×K	630.18	Joback Method
cpg	414.48	J/mol×K	658.60	Joback Method
cpg	424.88	J/mol×K	687.01	Joback Method
cpg	434.83	J/mol×K	715.43	Joback Method
cpg	444.32	J/mol×K	743.84	Joback Method
dvisc	0.0115627	Pa×s	309.17	Joback Method

dvisc	0.0030766	Pa×s	353.20	Joback Method
dvisc	0.0010979	Pa×s	397.23	Joback Method
dvisc	0.0004812	Pa×s	441.26	Joback Method
dvisc	0.0002450	Pa×s	485.29	Joback Method
dvisc	0.0001395	Pa×s	529.32	Joback Method
dvisc	0.0000867	Pa×s	573.35	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R319632&Units=SI

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