

methyl 4-hydroxyoctanoate

Inchi:	InChI=1S/C9H18O3/c1-3-4-5-8(10)6-7-9(11)12-2/h8,10H,3-7H2,1-2H3
InchiKey:	OBNCMDMTYZEKHM-UHFFFAOYSA-N
Formula:	C9H18O3
SMILES:	CCCCC(O)CCC(=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	1981.00		NIST Webbook
tb	573.35	K	Joback Method
tc	743.84	K	Joback Method
tf	309.17	K	Joback Method
vc	0.577	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	380.44	J/molxK	573.35	Joback Method
cpg	392.26	J/molxK	601.77	Joback Method
cpg	403.60	J/molxK	630.18	Joback Method
cpg	414.48	J/molxK	658.60	Joback Method
cpg	424.88	J/molxK	687.01	Joback Method
cpg	434.83	J/molxK	715.43	Joback Method
cpg	444.32	J/molxK	743.84	Joback Method
dvisc	0.0115627	Paxs	309.17	Joback Method
dvisc	0.0030766	Paxs	353.20	Joback Method

dvisc	0.0010979	Paxs	397.23	Joback Method
dvisc	0.0004812	Paxs	441.26	Joback Method
dvisc	0.0002450	Paxs	485.29	Joback Method
dvisc	0.0001395	Paxs	529.32	Joback Method
dvisc	0.0000867	Paxs	573.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R319612&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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