3-hydroxy-(E)-4-octen-2-one

Inchi: InChI=1S/C8H14O2/c1-3-4-5-6-8(10)7(2)9/h5-6,8,10H,3-4H2,1-2H3/b6-5+
InchiKey: VTTZYPRKOAQYNE-AATRIKPKSA-N
Formula: C8H14O2
SMILES: CCCC=CC(O)C(C)=O
Mol. weight [g/mol]: 142.20

Physical Properties

Property code	Value	Unit	Source
gf	-171.48	kJ/mol	Joback Method
hf	-361.32	kJ/mol	Joback Method
hfus	18.84	kJ/mol	Joback Method
hvap	56.40	kJ/mol	Joback Method
log10ws	-1.68		Crippen Method
logp	1.293		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
ripol	1683.00		NIST Webbook
tb	532.21	K	Joback Method
tc	711.46	K	Joback Method
tf	270.59	K	Joback Method
vc	0.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.27	J/mol×K	532.21	Joback Method
cpg	301.90	J/mol×K	562.08	Joback Method
cpg	312.01	J/mol×K	591.96	Joback Method
cpg	321.63	J/mol×K	621.83	Joback Method
cpg	330.78	J/mol×K	651.71	Joback Method
cpg	339.48	J/mol×K	681.58	Joback Method
cpg	347.75	J/mol×K	711.46	Joback Method
dvisc	0.0291030	Pa×s	270.59	Joback Method
dvisc	0.0061097	Pa×s	314.19	Joback Method

dvisc	0.0018764	Pa×s	357.80	Joback Method
dvisc	0.0007448	Pa×s	401.40	Joback Method
dvisc	0.0003543	Pa×s	445.00	Joback Method
dvisc	0.0001924	Pa×s	488.61	Joback Method
dvisc	0.0001155	Pa×s	532.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R241133&Units=SI
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

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