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

Inchi: InChI=1S/C7H12O2/c1-3-4-5-7(9)6(2)8/h4-5,7,9H,3H2,1-2H3/b5-4+
InchiKey: FHKIQZPHDMUUQU-SNAWJCMRSA-N
Formula: C7H12O2
SMILES: CCC=CC(O)C(C)=O
Mol. weight [g/mol]: 128.17

Physical Properties

Property code	Value	Unit	Source
gf	-179.90	kJ/mol	Joback Method
hf	-340.68	kJ/mol	Joback Method
hfus	16.25	kJ/mol	Joback Method
hvap	54.17	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	0.902		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
ripol	1586.00		NIST Webbook
ripol	1586.00		NIST Webbook
tb	509.33	K	Joback Method
tc	690.35	K	Joback Method
tf	259.32	K	Joback Method
vc	0.426	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.83	J/mol×K	509.33	Joback Method
cpg	257.53	J/mol×K	539.50	Joback Method
cpg	266.76	J/mol×K	569.67	Joback Method
cpg	275.53	J/mol×K	599.84	Joback Method
cpg	283.86	J/mol×K	630.01	Joback Method
cpg	291.77	J/mol×K	660.18	Joback Method
cpg	299.29	J/mol×K	690.35	Joback Method
dvisc	0.0362962	Pa×s	259.32	Joback Method

dvisc	0.0075170	Pa×s	300.99	Joback Method
dvisc	0.0022832	Pa×s	342.66	Joback Method
dvisc	0.0008979	Pa×s	384.33	Joback Method
dvisc	0.0004239	Pa×s	425.99	Joback Method
dvisc	0.0002287	Pa×s	467.66	Joback Method
dvisc	0.0001365	Pa×s	509.33	Joback Method

Sources

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=R241108&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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