

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

Inchi:	InChI=1S/C7H12O2/c1-3-4-5-7(9)6(2)8/h4-6,8H,3H2,1-2H3/b5-4+
InchiKey:	RGCWOHOTABNDBA-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
mvol	112.630	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
ripol	1619.00		NIST Webbook
ripol	1619.00		NIST Webbook
tb	509.33	K	Joback Method
tc	690.35	K	Joback Method
tf	259.32	K	Joback Method
vc	0.426	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.83	J/mol×K	509.33	Joback Method
cpg	291.77	J/mol×K	660.18	Joback Method
cpg	283.86	J/mol×K	630.01	Joback Method
cpg	275.53	J/mol×K	599.84	Joback Method
cpg	266.76	J/mol×K	569.67	Joback Method
cpg	257.53	J/mol×K	539.50	Joback Method
cpg	299.29	J/mol×K	690.35	Joback Method
dvisc	0.0001365	Paxs	509.33	Joback Method

dvisc	0.0002287	Paxs	467.66	Joback Method
dvisc	0.0004239	Paxs	425.99	Joback Method
dvisc	0.0008979	Paxs	384.33	Joback Method
dvisc	0.0022832	Paxs	342.66	Joback Method
dvisc	0.0075170	Paxs	300.99	Joback Method
dvisc	0.0362962	Paxs	259.32	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=R240932&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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