

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

Inchi:	InChI=1S/C8H14O2/c1-3-4-5-6-8(10)7(2)9/h5-7,9H,3-4H2,1-2H3/b6-5+
InchiKey:	UWPSVTSYXWNHHW-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	1698.00		NIST Webbook
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tb	532.21	K	Joback Method
tc	711.46	K	Joback Method
tf	270.59	K	Joback Method
vc	0.482	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.27	J/molxK	532.21	Joback Method
cpg	339.48	J/molxK	681.58	Joback Method
cpg	330.78	J/molxK	651.71	Joback Method
cpg	321.63	J/molxK	621.83	Joback Method
cpg	312.01	J/molxK	591.96	Joback Method
cpg	301.90	J/molxK	562.08	Joback Method
cpg	347.75	J/molxK	711.46	Joback Method
dvisc	0.0001155	Paxs	532.21	Joback Method

dvisc	0.0001924	Paxs	488.61	Joback Method
dvisc	0.0003543	Paxs	445.00	Joback Method
dvisc	0.0007448	Paxs	401.40	Joback Method
dvisc	0.0018764	Paxs	357.80	Joback Method
dvisc	0.0061097	Paxs	314.19	Joback Method
dvisc	0.0291030	Paxs	270.59	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=R240952&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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