

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

Inchi:	InChI=1S/C10H18O2/c1-3-4-5-6-7-8-10(12)9(2)11/h7-9,11H,3-6H2,1-2H3/b8-7+
InchiKey:	QGMOZIDHLFOEDQ-BQYQJAHWSA-N
Formula:	C10H18O2
SMILES:	CCCCC=CC(=O)C(C)O
Mol. weight [g/mol]:	170.25

Physical Properties

Property code	Value	Unit	Source
gf	-154.64	kJ/mol	Joback Method
hf	-402.60	kJ/mol	Joback Method
hfus	24.02	kJ/mol	Joback Method
hvap	60.85	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.073		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
ripol	1959.00		NIST Webbook
ripol	1959.00		NIST Webbook
tb	577.97	K	Joback Method
tc	754.09	K	Joback Method
tf	293.13	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.58	J/molxK	577.97	Joback Method
cpg	395.79	J/molxK	607.32	Joback Method
cpg	407.43	J/molxK	636.68	Joback Method
cpg	418.50	J/molxK	666.03	Joback Method
cpg	429.05	J/molxK	695.38	Joback Method
cpg	439.09	J/molxK	724.73	Joback Method
cpg	448.64	J/molxK	754.09	Joback Method
dvisc	0.0187361	Paxs	293.13	Joback Method

dvisc	0.0040298	Paxs	340.60	Joback Method
dvisc	0.0012624	Paxs	388.08	Joback Method
dvisc	0.0005093	Paxs	435.55	Joback Method
dvisc	0.0002456	Paxs	483.02	Joback Method
dvisc	0.0001350	Paxs	530.50	Joback Method
dvisc	0.0000818	Paxs	577.97	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=R240927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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