

(E)-4-Oxo-2-hexenal

Other names:	(E)-4-Oxo-hex-2-enal
Inchi:	InChI=1S/C6H8O2/c1-2-6(8)4-3-5-7/h3-5H,2H2,1H3/b4-3+
InchiKey:	GVKYFODEMNLGS-ONEGZZNKSA-N
Formula:	C6H8O2
SMILES:	CCC(=O)C=CC=O
Mol. weight [g/mol]:	112.13

Physical Properties

Property code	Value	Unit	Source
gf	-148.58	kJ/mol	Joback Method
hf	-248.11	kJ/mol	Joback Method
hfus	15.39	kJ/mol	Joback Method
hvap	42.37	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	0.721		Crippen Method
mcpvol	94.240	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	976.00		NIST Webbook
rinpol	958.00		NIST Webbook
rinpol	958.00		NIST Webbook
tb	443.37	K	Joback Method
tc	637.17	K	Joback Method
tf	244.23	K	Joback Method
vc	0.374	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.07	J/mol×K	443.37	Joback Method
cpg	187.79	J/mol×K	475.67	Joback Method
cpg	196.05	J/mol×K	507.97	Joback Method
cpg	203.86	J/mol×K	540.27	Joback Method
cpg	211.24	J/mol×K	572.57	Joback Method
cpg	218.21	J/mol×K	604.87	Joback Method

cpg	224.80	J/mol×K	637.17	Joback Method
dvisc	0.0034701	Paxs	244.23	Joback Method
dvisc	0.0018442	Paxs	277.42	Joback Method
dvisc	0.0011219	Paxs	310.61	Joback Method
dvisc	0.0007512	Paxs	343.80	Joback Method
dvisc	0.0005398	Paxs	376.99	Joback Method
dvisc	0.0004092	Paxs	410.18	Joback Method
dvisc	0.0003233	Paxs	443.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R571429&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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