(E)-4-Oxohex-2-enal

Other names: (E)-4-Oxo-2-hexenal
Inchi: InChI=1S/C6H8O2/c1-2-6(8)4-3-5-7/h3-5H,2H2,1H3/b4-3+
InchiKey: GVKYFODEMNCLGS-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
mcvol	94.240	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
rinpol	958.00		NIST Webbook
rinpol	958.00		NIST Webbook
ripol	1599.00		NIST Webbook
ripol	1599.00		NIST Webbook
tb	443.37	K	Joback Method
tc	637.17	K	Joback Method
tf	244.23	K	Joback Method
vc	0.374	m3/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	Pa×s	244.23	Joback Method
dvisc	0.0018442	Pa×s	277.42	Joback Method
dvisc	0.0011219	Pa×s	310.61	Joback Method
dvisc	0.0007512	Pa×s	343.80	Joback Method
dvisc	0.0005398	Pa×s	376.99	Joback Method
dvisc	0.0004092	Pa×s	410.18	Joback Method
dvisc	0.0003233	Pa×s	443.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374042&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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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