

Hexa-2,4-dienal

Other names:	2,4-Hexadienal 2,4-Hexadien-1-al
Inchi:	InChI=1S/C6H8O/c1-2-3-4-5-6-7/h2-6H,1H3/b3-2+,5-4+
InchiKey:	BATOPA ZDIZEVQF-MQQKCMAXSA-N
Formula:	C6H8O
SMILES:	CC=CC=CC=O
Mol. weight [g/mol]:	96.13
CAS:	80466-34-8

Physical Properties

Property code	Value	Unit	Source
gf	60.56	kJ/mol	Joback Method
hf	-18.31	kJ/mol	Joback Method
hfus	13.99	kJ/mol	Joback Method
hvap	35.59	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.318		Crippen Method
mvol	88.370	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
rinpol	879.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	910.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	892.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	872.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	915.00		NIST Webbook
rinpol	907.00		NIST Webbook

rinpol	887.00		NIST Webbook
rinpol	889.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	899.00		NIST Webbook
rinpol	911.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1406.00		NIST Webbook
ripol	1408.00		NIST Webbook
ripol	1441.00		NIST Webbook
ripol	1402.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1368.00		NIST Webbook
tb	393.66	K	Joback Method
tc	584.72	K	Joback Method
tf	189.22	K	Joback Method
vc	0.348	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.61	J/molxK	393.66	Joback Method
cpg	189.99	J/molxK	552.88	Joback Method
cpg	182.88	J/molxK	521.04	Joback Method
cpg	175.32	J/molxK	489.19	Joback Method
cpg	167.28	J/molxK	457.35	Joback Method
cpg	158.72	J/molxK	425.50	Joback Method
cpg	196.67	J/molxK	584.72	Joback Method
dvisc	0.0002152	Paxs	393.66	Joback Method
dvisc	0.0002751	Paxs	359.59	Joback Method
dvisc	0.0003703	Paxs	325.51	Joback Method
dvisc	0.0005342	Paxs	291.44	Joback Method
dvisc	0.0008493	Paxs	257.37	Joback Method
dvisc	0.0015554	Paxs	223.29	Joback Method
dvisc	0.0035420	Paxs	189.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C80466348&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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