(E,E)-2,4-Hexadienal

Inchi: InChI=1S/C6H8O/c1-2-3-4-5-6-7/h2-6H,1H3/b3-2+,5-4+
InchiKey: BATOPAZDIZEVQF-MQQKCMAXSA-N
Formula: C6H8O
SMILES: CC=CC=CC=O
Mol. weight [g/mol]: 96.13

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
mcvol	88.370	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
rinpol	911.00		NIST Webbook
rinpol	913.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	907.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	917.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1395.00		NIST Webbook
tb	393.66	K	Joback Method
tc	584.72	K	Joback Method
tf	189.22	K	Joback Method
vc	0.348	m3/kmol	Joback Method

Temperature Dependent Properties

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

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R615415&Units=SI

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