

Hexanal, 5-methyl-

Other names:	5-Methylhexan-1-al 5-Methyl hexanal
Inchi:	InChI=1S/C7H14O/c1-7(2)5-3-4-6-8/h6-7H,3-5H2,1-2H3
InchiKey:	GEKRISJWBAlIAA-UHFFFAOYSA-N
Formula:	C7H14O
SMILES:	CC(C)CCCC=O
Mol. weight [g/mol]:	114.19
CAS:	1860-39-5

Physical Properties

Property code	Value	Unit	Source
gf	-93.90	kJ/mol	Joback Method
hf	-278.67	kJ/mol	Joback Method
hfus	12.65	kJ/mol	Joback Method
hvap	37.51	kJ/mol	Joback Method
log10ws	-1.79		Crippen Method
logp	2.012		Crippen Method
mvol	111.060	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
ripol	1150.00		NIST Webbook
tb	407.78	K	Joback Method
tc	583.42	K	Joback Method
tf	195.65	K	Joback Method
vc	0.439	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.97	J/molxK	407.78	Joback Method
cpg	269.38	J/molxK	554.14	Joback Method
cpg	259.76	J/molxK	524.87	Joback Method
cpg	249.71	J/molxK	495.60	Joback Method
cpg	239.24	J/molxK	466.33	Joback Method
cpg	228.33	J/molxK	437.05	Joback Method

cpg	278.60	J/mol×K	583.42	Joback Method
dvisc	0.0003089	Paxs	407.78	Joback Method
dvisc	0.0004085	Paxs	372.42	Joback Method
dvisc	0.0005728	Paxs	337.07	Joback Method
dvisc	0.0008693	Paxs	301.72	Joback Method
dvisc	0.0014738	Paxs	266.36	Joback Method
dvisc	0.0029368	Paxs	231.00	Joback Method
dvisc	0.0075086	Paxs	195.65	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=C1860395&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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