

3-Hexenoic acid, methyl ester, (Z)-

Other names:	Z-Methyl 3-hexenoate Methyl (3Z)-3-hexenoate Methyl (Z)-3-hexenoate 3-Hexenoic acid, methyl ester, (3Z)- methyl (Z)-hex-3-enoate
Inchi:	InChI=1S/C7H12O2/c1-3-4-5-6-7(8)9-2/h4-5H,3,6H2,1-2H3/b5-4-
InchiKey:	XEAIHUDTEINXFG-PLNGDYQASA-N
Formula:	C7H12O2
SMILES:	CCC=CCC(=O)OC
Mol. weight [g/mol]:	128.17
CAS:	13894-62-7

Physical Properties

Property code	Value	Unit	Source
gf	-145.64	kJ/mol	Joback Method
hf	-315.39	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	40.29	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	1.516		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
rinpol	917.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	933.00		NIST Webbook
ripol	1260.00		NIST Webbook
ripol	1265.00		NIST Webbook
ripol	1252.00		NIST Webbook
ripol	1253.00		NIST Webbook
tb	440.01	K	Joback Method
tc	625.03	K	Joback Method
tf	235.73	K	Joback Method
vc	0.431	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.68	J/molxK	440.01	Joback Method
cpg	233.44	J/molxK	470.85	Joback Method
cpg	243.76	J/molxK	501.68	Joback Method
cpg	253.64	J/molxK	532.52	Joback Method
cpg	263.10	J/molxK	563.36	Joback Method
cpg	272.15	J/molxK	594.20	Joback Method
cpg	280.80	J/molxK	625.03	Joback Method
dvisc	0.0029377	Paxs	235.73	Joback Method
dvisc	0.0014537	Paxs	269.78	Joback Method
dvisc	0.0008422	Paxs	303.82	Joback Method
dvisc	0.0005447	Paxs	337.87	Joback Method
dvisc	0.0003815	Paxs	371.92	Joback Method
dvisc	0.0002837	Paxs	405.96	Joback Method
dvisc	0.0002208	Paxs	440.01	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C13894627&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

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