cis-3-Hexenal diethyl acetal

Other names:	3-Hexene, 1,1-diethoxy-, (Z)- cis-1,1-Diethoxy-3-hexene (3Z)-1,1-Diethoxy-3-hexene (Z)-3-Hexenal diethyl acetal 3-Hexene, 1,1-diethoxy-, (3Z)- (Z)-1,1-diethoxyhex-3-ene
Inchi:	InChI=1S/C10H20O2/c1-4-7-8-9-10(11-5-2)12-6-3/h7-8,10H,4-6,9H2,1-3H3/b8-7-
InchiKey:	IOBHVJHSBREPFR-FPLPWBNLSA-N
Formula:	C10H20O2
SMILES:	CCC=CCC(OCC)OCC
Mol. weight [g/mol]:	172.26
CAS:	73545-18-3

Physical Properties

Property code	Value	Unit	Source
gf	-98.90	kJ/mol	Joback Method
hf	-402.23	kJ/mol	Joback Method
hfus	20.71	kJ/mol	Joback Method
hvap	42.24	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.742		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
ripol	1272.00		NIST Webbook
ripol	1269.00		NIST Webbook
ripol	1269.00		NIST Webbook
ripol	1272.00		NIST Webbook
tb	476.76	K	Joback Method
tc	650.07	K	Joback Method
tf	226.84	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.11	J/mol×K	476.76	Joback Method
cpg	421.20	J/mol×K	621.18	Joback Method
cpg	408.61	J/mol×K	592.30	Joback Method
cpg	395.52	J/mol×K	563.41	Joback Method
cpg	381.91	J/mol×K	534.53	Joback Method
cpg	367.77	J/mol×K	505.64	Joback Method
cpg	433.28	J/mol×K	650.07	Joback Method
dvisc	0.0001354	Pa×s	476.76	Joback Method
dvisc	0.0001834	Pa×s	435.11	Joback Method
dvisc	0.0002648	Pa×s	393.45	Joback Method
dvisc	0.0004172	Pa×s	351.80	Joback Method
dvisc	0.0007426	Pa×s	310.15	Joback Method
dvisc	0.0015806	Pa×s	268.49	Joback Method
dvisc	0.0044403	Pa×s	226.84	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=C73545183&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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https://www.chemeo.com/cid/76-902-6/cis-3-Hexenal-diethyl-acetal.pdf

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