

2-Hexoxy acetaldehyde dimethyl acetal

Other names:	1-(2,2-dimethoxyethoxy)hexane 2-Hexoxyacetaldehyde dimethylacetal Acetaldehyde, (hexyloxy)-, dimethyl acetal Ethane, 1,1-dimethoxy-2-hexyloxy Hexoxyacetaldehyde dimethylacetal «beta»-Hexoxyacetaldehyde dimethylacetal
Inchi:	InChI=1S/C10H22O3/c1-4-5-6-7-8-13-9-10(11-2)12-3/h10H,4-9H2,1-3H3
InchiKey:	LIVMHHPZBYEKCUCUHFFFAOYSA-N
Formula:	C10H22O3
SMILES:	CCCCCOC(OC)OC
Mol. weight [g/mol]:	190.28

Physical Properties

Property code	Value	Unit	Source
af	0.5781		Cheméo Relay (1.0)
gf	-284.12	kJ/mol	Joback Method
hf	-633.48	kJ/mol	Cheméo Relay (1.0)
hfus	21.70	kJ/mol	Joback Method
hvap	59.49	kJ/mol	Cheméo Relay (1.0)
ie	9.55	eV	Cheméo Relay (1.0)
log10ws	-1.92		Cheméo Relay (1.0)
logp	2.202		Crippen Method
mcvol	169.370	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1234.00		NIST Webbook
ripol	1528.00		NIST Webbook
tb	484.19	K	Cheméo Relay (1.0)
tc	647.79	K	Cheméo Relay (1.0)
tf	211.05	K	Cheméo Relay (1.0)
vc	0.642	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	396.28	J/mol×K	495.02	Joback Method
cpg	410.97	J/mol×K	522.64	Joback Method
cpg	425.24	J/mol×K	550.26	Joback Method
cpg	439.07	J/mol×K	577.87	Joback Method
cpg	452.46	J/mol×K	605.49	Joback Method
cpg	465.40	J/mol×K	633.11	Joback Method
cpg	477.89	J/mol×K	660.73	Joback Method
dvisc	0.0031538	Pa×s	254.15	Joback Method
dvisc	0.0012966	Pa×s	294.30	Joback Method
dvisc	0.0006598	Pa×s	334.44	Joback Method
dvisc	0.0003881	Pa×s	374.58	Joback Method
dvisc	0.0002530	Pa×s	414.73	Joback Method
dvisc	0.0001778	Pa×s	454.88	Joback Method
dvisc	0.0001324	Pa×s	495.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17597954&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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