

(E)-2-hexenal diethyl acetal

Other names:	(E)-1,1-diethoxyhex-2-ene
Inchi:	InChI=1S/C10H20O2/c1-4-7-8-9-10(11-5-2)12-6-3/h8-10H,4-7H2,1-3H3/b9-8+
InchiKey:	WMQKYHTZGYIHHD-CMDGGOBGS-A-N
Formula:	C10H20O2
SMILES:	CCCC=CC(OCC)OCC
Mol. weight [g/mol]:	172.26
CAS:	67746-30-9

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	1287.00		NIST Webbook
ripol	1287.00		NIST Webbook
ripol	1285.00		NIST Webbook
ripol	1285.00		NIST Webbook
tb	476.76	K	Joback Method
tc	650.07	K	Joback Method
tf	226.84	K	Joback Method
vc	0.606	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.11	J/molxK	476.76	Joback Method
cpg	367.77	J/molxK	505.64	Joback Method
cpg	381.91	J/molxK	534.53	Joback Method
cpg	395.52	J/molxK	563.41	Joback Method

cpg	408.61	J/mol×K	592.30	Joback Method
cpg	421.20	J/mol×K	621.18	Joback Method
cpg	433.28	J/mol×K	650.07	Joback Method
dvisc	0.0044403	Paxs	226.84	Joback Method
dvisc	0.0015806	Paxs	268.49	Joback Method
dvisc	0.0007426	Paxs	310.15	Joback Method
dvisc	0.0004172	Paxs	351.80	Joback Method
dvisc	0.0002648	Paxs	393.45	Joback Method
dvisc	0.0001834	Paxs	435.11	Joback Method
dvisc	0.0001354	Paxs	476.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67746309&Units=SI
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

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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