

3,5-Dimethoxy-1-hexanol

Inchi:	InChI=1S/C8H18O3/c1-7(10-2)6-8(11-3)4-5-9/h7-9H,4-6H2,1-3H3
InchiKey:	NXAYPXAJVWIOV-UHFFFAOYSA-N
Formula:	C8H18O3
SMILES:	COC(C)CC(CCO)OC
Mol. weight [g/mol]:	162.23
CAS:	90952-10-6

Physical Properties

Property code	Value	Unit	Source
gf	-335.22	kJ/mol	Joback Method
hf	-635.68	kJ/mol	Joback Method
hfus	15.89	kJ/mol	Joback Method
hvap	54.12	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.809		Crippen Method
mcvol	141.190	ml/mol	McGowan Method
pc	2735.42	kPa	Joback Method
tb	518.58	K	Joback Method
tc	684.36	K	Joback Method
tf	255.20	K	Joback Method
vc	0.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.69	J/molxK	518.58	Joback Method
cpg	394.94	J/molxK	656.73	Joback Method
cpg	384.68	J/molxK	629.10	Joback Method
cpg	374.02	J/molxK	601.47	Joback Method
cpg	362.96	J/molxK	573.84	Joback Method
cpg	351.52	J/molxK	546.21	Joback Method
cpg	404.81	J/molxK	684.36	Joback Method
dvisc	0.0000880	Paxs	518.58	Joback Method
dvisc	0.0001531	Paxs	474.68	Joback Method

dvisc	0.0002979	Paxs	430.79	Joback Method
dvisc	0.0006747	Paxs	386.89	Joback Method
dvisc	0.0018832	Paxs	342.99	Joback Method
dvisc	0.0071048	Paxs	299.10	Joback Method
dvisc	0.0423244	Paxs	255.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90952106&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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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