HEPTANAL, 7,7-DIMETHOXY-

Inchi: InChI=1S/C9H18O3/c1-11-9(12-2)7-5-3-4-6-8-10/h8-9H,3-7H2,1-2H3
InchiKey: ZSCWUFCWRFKZGG-UHFFFAOYSA-N
Formula: C9H18O3
SMILES: COC(CCCCCC=O)OC
Mol. weight [g/mol]: 174.24

Physical Properties

Property code	Value	Unit	Source
af	0.5587		Cheméo Relay (1.0)
hf	-578.81	kJ/mol	Cheméo Relay (1.0)
hfus	20.21	kJ/mol	Joback Method
hvap	58.52	kJ/mol	Cheméo Relay (1.0)
ie	9.30	eV	Cheméo Relay (1.0)
log10ws	-0.75		Cheméo Relay (1.0)
logp	1.755		Crippen Method
mcvol	150.980	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
tb	501.42	K	Cheméo Relay (1.0)
tc	674.43	K	Cheméo Relay (1.0)
tf	246.37	K	Cheméo Relay (1.0)
vc	0.557	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.06	J/mol×K	498.38	Joback Method
cpg	420.71	J/mol×K	670.88	Joback Method
cpg	409.89	J/mol×K	642.13	Joback Method
cpg	398.61	J/mol×K	613.38	Joback Method
cpg	386.89	J/mol×K	584.63	Joback Method
cpg	374.72	J/mol×K	555.88	Joback Method
cpg	362.11	J/mol×K	527.13	Joback Method
dvisc	0.0005630	Pa×s	380.51	Joback Method
dvisc	0.0002041	Pa×s	498.38	Joback Method

dvisc	0.0002701	Pa×s	459.09	Joback Method
dvisc	0.0003768	Pa×s	419.80	Joback Method
dvisc	0.0038602	Pa×s	262.65	Joback Method
dvisc	0.0009226	Pa×s	341.23	Joback Method
dvisc	0.0017194	Pa×s	301.94	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60090779&Units=SI

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume