Heptane, 1,1-dimethoxy-

Other names: Heptanal, dimethyl acetal
1,1-Dimethoxyheptane
n-Heptanal dimethyl acetal
Inchi: InChI=1S/C9H20O2/c1-4-5-6-7-8-9(10-2)11-3/h9H,4-8H2,1-3H3
InchiKey: BBMCNYFBAIUERL-UHFFFAOYSA-N
Formula: C9H20O2
SMILES: CCCCCCC(OC)OC
Mol. weight [g/mol]: 160.25
CAS: 10032-05-0

Physical Properties

Property code	Value	Unit	Source
gf	-187.54	kJ/mol	Joback Method
hf	-498.81	kJ/mol	Joback Method
hfus	17.92	kJ/mol	Joback Method
hvap	40.06	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	2.576		Crippen Method
mcvol	149.410	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1080.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1063.00		NIST Webbook
rinpol	1069.00		NIST Webbook
ripol	1261.00		NIST Webbook
ripol	1265.00		NIST Webbook
tb	449.72	K	Joback Method
tc	616.59	K	Joback Method
tf	220.65	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	324.83	J/mol×K	449.72	Joback Method
cpg	338.74	J/mol×K	477.53	Joback Method
cpg	352.24	J/mol×K	505.34	Joback Method
cpg	365.32	J/mol×K	533.15	Joback Method
cpg	377.99	J/mol×K	560.97	Joback Method
cpg	390.23	J/mol×K	588.78	Joback Method
cpg	402.06	J/mol×K	616.59	Joback Method
dvisc	0.0048122	Pa×s	220.65	Joback Method
dvisc	0.0018379	Pa×s	258.83	Joback Method
dvisc	0.0008990	Pa×s	297.01	Joback Method
dvisc	0.0005175	Pa×s	335.19	Joback Method
dvisc	0.0003336	Pa×s	373.36	Joback Method
dvisc	0.0002332	Pa×s	411.54	Joback Method
dvisc	0.0001733	Pa×s	449.72	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C10032050&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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