Heptane, 1,1-diethoxy-

Other names:	Heptanal, diethyl acetal
	Heptaldehyde diethyl acetal
	1,1-Diethoxyheptane
	n-Heptanal diethyl acetal
Inchi:	InChI=1S/C11H24O2/c1-4-7-8-9-10-11(12-5-2)13-6-3/h11H,4-10H2,1-3H3
InchiKey:	UGOCNHASEZIJFQ-UHFFFAOYSA-N
Formula:	C11H24O2
SMILES:	CCCCCCC(OCC)OCC
Mol. weight [g/mol]:	188.31
CAS:	688-82-4

Physical Properties

Property code	Value	Unit	Source
gf	-170.70	kJ/mol	Joback Method
hf	-540.09	kJ/mol	Joback Method
hfus	23.10	kJ/mol	Joback Method
hvap	44.51	kJ/mol	Joback Method
log10ws	-3.21		Crippen Method
logp	3.356		Crippen Method
mcvol	177.590	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	1179.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1340.00		NIST Webbook
ripol	1334.00		NIST Webbook
ripol	1319.00		NIST Webbook
tb	482.00 ± 5.00	K	NIST Webbook
tc	660.38	K	Joback Method
tf	243.19	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	416.01	J/mol×K	495.48	Joback Method
cpg	489.68	J/mol×K	632.90	Joback Method
cpg	475.97	J/mol×K	605.41	Joback Method
cpg	461.75	J/mol×K	577.93	Joback Method
cpg	447.02	J/mol×K	550.45	Joback Method
cpg	431.77	J/mol×K	522.96	Joback Method
cpg	502.88	J/mol×K	660.38	Joback Method
dvisc	0.0001488	Pa×s	495.48	Joback Method
dvisc	0.0002018	Pa×s	453.43	Joback Method
dvisc	0.0002913	Pa×s	411.38	Joback Method
dvisc	0.0004572	Pa×s	369.34	Joback Method
dvisc	0.0008055	Pa×s	327.29	Joback Method
dvisc	0.0016771	Pa×s	285.24	Joback Method
dvisc	0.0044998	Pa×s	243.19	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C688824&Units=SI

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