UNDECANE, 1,1-DIMETHOXY-

Other names: Undecane, 1,1-dimethoxy-
Inchi: InChI=1S/C13H28O2/c1-4-5-6-7-8-9-10-11-12-13(14-2)15-3/h13H,4-12H2,1-3H3
InchiKey: FBJUQTUWWCVIDH-UHFFFAOYSA-N
Formula: C13H28O2
SMILES: CCCCCCCCCCC(OC)OC
Mol. weight [g/mol]: 216.37

Physical Properties

Property code	Value	Unit	Source
af	0.6439		Cheméo Relay (1.0)
gf	-153.86	kJ/mol	Joback Method
hf	-572.62	kJ/mol	Cheméo Relay (1.0)
hfus	28.28	kJ/mol	Joback Method
hvap	66.99	kJ/mol	Cheméo Relay (1.0)
ie	9.45	eV	Cheméo Relay (1.0)
log10ws	-4.53		Cheméo Relay (1.0)
logp	4.136		Crippen Method
mcvol	205.770	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1668.00		NIST Webbook
tb	519.03	K	Cheméo Relay (1.0)
tc	677.40	K	Cheméo Relay (1.0)
tf	242.85	K	Cheméo Relay (1.0)
vc	0.796	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.89	J/mol×K	541.24	Joback Method
cpg	532.12	J/mol×K	568.43	Joback Method
cpg	548.75	J/mol×K	595.63	Joback Method

cpg	564.78	J/mol×K	622.82	Joback Method
cpg	580.21	J/mol×K	650.02	Joback Method
cpg	595.06	J/mol×K	677.21	Joback Method
cpg	609.31	J/mol×K	704.41	Joback Method
dvisc	0.0039976	Pa×s	265.73	Joback Method
dvisc	0.0014601	Pa×s	311.65	Joback Method
dvisc	0.0006907	Pa×s	357.57	Joback Method
dvisc	0.0003874	Pa×s	403.49	Joback Method
dvisc	0.0002446	Pa×s	449.40	Joback Method
dvisc	0.0001681	Pa×s	495.32	Joback Method
dvisc	0.0001232	Pa×s	541.24	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=C52517676&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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