METHYL DECYL ETHER

Other names:	Decane, 1-methoxy-
	Ether, decyl methyl
	Decyl methyl ether
	Methyl decyl ether
	Methyl n-decyl ether
Inchi:	InChI=1S/C11H24O/c1-3-4-5-6-7-8-9-10-11-12-2/h3-11H2,1-2H3
InchiKey:	JPEWDCTZJFUITH-UHFFFAOYSA-N
Formula:	C11H24O
SMILES:	CCCCCCCCCCOC
Mol. weight [g/mol]:	172.31

Physical Properties

Property code	Value	Unit	Source
af	0.5842		Cheméo Relay (1.0)
chl	-7315.18	kJ/mol	NIST Webbook
gf	-63.26	kJ/mol	Joback Method
hf	-381.10 ± 2.10	kJ/mol	NIST Webbook
hfl	-443.40 ± 2.10	kJ/mol	NIST Webbook
hfus	25.43	kJ/mol	Joback Method
hvap	62.30 ± 0.30	kJ/mol	NIST Webbook
hvap	62.30 ± 0.30	kJ/mol	NIST Webbook
hvap	62.30	kJ/mol	NIST Webbook
hvap	62.60	kJ/mol	NIST Webbook
ie	9.45	eV	Cheméo Relay (1.0)
log10ws	-4.50		Cheméo Relay (1.0)
logp	3.773		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	1905.24	kPa	Joback Method
rinpol	1227.30		NIST Webbook
sl	490.50	J/mol×K	NIST Webbook
tb	477.97	K	Cheméo Relay (1.0)
tc	646.98	K	Cheméo Relay (1.0)
tf	255.13	K	Cheméo Relay (1.0)
tt	243.42 ± 0.07	K	NIST Webbook
vc	0.671	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	474.10	J/mol×K	635.31	Joback Method
cpg	447.47	J/mol×K	581.37	Joback Method
cpg	433.40	J/mol×K	554.41	Joback Method
cpg	461.04	J/mol×K	608.34	Joback Method
cpg	388.04	J/mol×K	473.50	Joback Method
cpg	403.69	J/mol×K	500.47	Joback Method
cpg	418.81	J/mol×K	527.44	Joback Method
cpl	370.80	J/mol×K	298.15	NIST Webbook
cpl	370.50	J/mol×K	298.15	NIST Webbook
dvisc	0.0003548	Pa×s	394.32	Joback Method
dvisc	0.0005375	Pa×s	354.73	Joback Method
dvisc	0.0043175	Pa×s	235.96	Joback Method
dvisc	0.0001903	Pa×s	473.50	Joback Method
dvisc	0.0009041	Pa×s	315.14	Joback Method
dvisc	0.0017659	Pa×s	275.55	Joback Method
dvisc	0.0002526	Pa×s	433.91	Joback Method
hfust	31.71	kJ/mol	243.50	NIST Webbook
hfust	31.71	kJ/mol	243.50	NIST Webbook
hfust	31.72	kJ/mol	243.47	NIST Webbook
hvapt	56.90	kJ/mol	385.00	NIST Webbook
hvapt	57.00	kJ/mol	406.00	NIST Webbook
hvapt	45.50	kJ/mol	406.00	NIST Webbook
sfust	130.31	J/mol×K	243.47	NIST Webbook

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=C7289523&Units=SI

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume