Methyl undecyl ether

Inchi:	InChI=1S/C12H26O/c1-3-4-5-6-7-8-9-10-11-12-13-2/h3-12H2,1-2H3
InchiKey:	FBLLWAUEWCBESD-UHFFFAOYSA-N
Formula:	C12H26O
SMILES:	CCCCCCCCCCCOC
Mol. weight [g/mol]:	186.33
CAS:	7289-53-4

Physical Properties

Property code	Value	Unit	Source
gf	-54.84	kJ/mol	Joback Method
hf	-423.23	kJ/mol	Joback Method
hfus	28.02	kJ/mol	Joback Method
hvap	44.72	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	4.164		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	1318.00		NIST Webbook
rinpol	1325.00		NIST Webbook
rinpol	1318.00		NIST Webbook
ripol	1453.00		NIST Webbook
tb	496.38	K	Joback Method
tc	657.41	K	Joback Method
tf	247.23	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.65	J/mol×K	496.38	Joback Method
cpg	512.19	J/mol×K	630.57	Joback Method
cpg	497.99	J/mol×K	603.73	Joback Method
cpg	483.25	J/mol×K	576.89	Joback Method
cpg	467.95	J/mol×K	550.06	Joback Method

cpg	452.08	J/mol×K	523.22	Joback Method
cpg	525.85	J/mol×K	657.41	Joback Method
dvisc	0.0001768	Pa×s	496.38	Joback Method
dvisc	0.0002356	Pa×s	454.86	Joback Method
dvisc	0.0003327	Pa×s	413.33	Joback Method
dvisc	0.0005075	Pa×s	371.80	Joback Method
dvisc	0.0008607	Pa×s	330.28	Joback Method
dvisc	0.0016995	Pa×s	288.75	Joback Method
dvisc	0.0042171	Pa×s	247.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7289534&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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