

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:	FBLWUAUEWCBESD-UHFFFAOYSA-N
Formula:	C12H26O
SMILES:	CCCCCCCCCCCCOC
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	1325.00		NIST Webbook
rinpol	1318.00		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/molxK	496.38	Joback Method
cpg	452.08	J/molxK	523.22	Joback Method
cpg	467.95	J/molxK	550.06	Joback Method
cpg	483.25	J/molxK	576.89	Joback Method
cpg	497.99	J/molxK	603.73	Joback Method

cpg	512.19	J/molxK	630.57	Joback Method
cpg	525.85	J/molxK	657.41	Joback Method
dvisc	0.0042171	Paxs	247.23	Joback Method
dvisc	0.0016995	Paxs	288.75	Joback Method
dvisc	0.0008607	Paxs	330.28	Joback Method
dvisc	0.0005075	Paxs	371.80	Joback Method
dvisc	0.0003327	Paxs	413.33	Joback Method
dvisc	0.0002356	Paxs	454.86	Joback Method
dvisc	0.0001768	Paxs	496.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C7289534&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

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