

Dodecane, 1-methoxy-

Other names:	1-methoxydodecane methyl dodecyl ether
Inchi:	InChI=1S/C13H28O/c1-3-4-5-6-7-8-9-10-11-12-13-14-2/h3-13H2,1-2H3
InchiKey:	JWCACDSKXWPOFF-UHFFFAOYSA-N
Formula:	C13H28O
SMILES:	CCCCCCCCCCCCOC
Mol. weight [g/mol]:	200.36
CAS:	3482-63-1

Physical Properties

Property code	Value	Unit	Source
gf	-46.42	kJ/mol	Joback Method
hf	-443.87	kJ/mol	Joback Method
hfus	30.61	kJ/mol	Joback Method
hvap	46.94	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	4.554		Crippen Method
mcvol	199.900	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpola	1424.10		NIST Webbook
rinpola	1424.10		NIST Webbook
tb	519.26	K	Joback Method
tc	679.58	K	Joback Method
tf	258.50	K	Joback Method
vc	0.781	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.12	J/mol×K	519.26	Joback Method
cpg	502.25	J/mol×K	545.98	Joback Method
cpg	518.78	J/mol×K	572.70	Joback Method
cpg	534.71	J/mol×K	599.42	Joback Method
cpg	550.05	J/mol×K	626.14	Joback Method

cpg	564.81	J/molxK	652.86	Joback Method
cpg	579.00	J/molxK	679.58	Joback Method
dvisc	0.0040611	Paxs	258.50	Joback Method
dvisc	0.0016146	Paxs	301.96	Joback Method
dvisc	0.0008096	Paxs	345.42	Joback Method
dvisc	0.0004737	Paxs	388.88	Joback Method
dvisc	0.0003087	Paxs	432.34	Joback Method
dvisc	0.0002175	Paxs	475.80	Joback Method
dvisc	0.0001625	Paxs	519.26	Joback Method

Sources

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=C3482631&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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