METHYL DODECYL ETHER

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]: 200.37

Physical Properties

Property code	Value	Unit	Source
af	0.6568		Cheméo Relay (1.0)
gf	-46.42	kJ/mol	Joback Method
hf	-434.28	kJ/mol	Cheméo Relay (1.0)
hfus	30.61	kJ/mol	Joback Method
hvap	69.78	kJ/mol	Cheméo Relay (1.0)
ie	9.50	eV	Cheméo Relay (1.0)
log10ws	-5.42		Cheméo Relay (1.0)
logp	4.554		Crippen Method
mcvol	199.900	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	1424.10		NIST Webbook
rinpol	1424.10		NIST Webbook
tb	512.85	K	Cheméo Relay (1.0)
tc	679.72	K	Cheméo Relay (1.0)
tf	273.03	K	Cheméo Relay (1.0)
vc	0.787	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.12	J/mol×K	519.26	Joback Method
cpg	579.00	J/mol×K	679.58	Joback Method
cpg	564.81	J/mol×K	652.86	Joback Method
cpg	550.05	J/mol×K	626.14	Joback Method

cpg	534.71	J/mol×K	599.42	Joback Method
cpg	518.78	J/mol×K	572.70	Joback Method
cpg	502.25	J/mol×K	545.98	Joback Method
dvisc	0.0004737	Pa×s	388.88	Joback Method
dvisc	0.0001625	Pa×s	519.26	Joback Method
dvisc	0.0002175	Pa×s	475.80	Joback Method
dvisc	0.0003087	Pa×s	432.34	Joback Method
dvisc	0.0040611	Pa×s	258.50	Joback Method
dvisc	0.0008096	Pa×s	345.42	Joback Method
dvisc	0.0016146	Pa×s	301.96	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3482631&Units=SI

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):

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume