Cyclododecyl methyl ether

Other names:	Cyclododecane, methoxy- methoxycyclododecane
Inchi:	InChI=1S/C13H26O/c1-14-13-11-9-7-5-3-2-4-6-8-10-12-13/h13H,2-12H2,1H3
InchiKey:	WDSOYUINLRIGNV-UHFFFAOYSA-N
Formula:	C13H26O
SMILES:	COC1CCCCCCCCCCC1
Mol. weight [g/mol]:	198.34
CAS:	2986-54-1

Physical Properties

Property code	Value	Unit	Source
gf	-94.57	kJ/mol	Joback Method
hf	-426.51	kJ/mol	Joback Method
hfus	9.85	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	4.306		Crippen Method
mcvol	189.040	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
tb	564.43	K	Joback Method
tc	796.88	K	Joback Method
tf	244.76	K	Joback Method
vc	0.666	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.15	J/mol×K	564.43	Joback Method
cpg	514.02	J/mol×K	603.17	Joback Method
cpg	540.32	J/mol×K	641.91	Joback Method
cpg	565.02	J/mol×K	680.65	Joback Method
cpg	588.11	J/mol×K	719.40	Joback Method
cpg	609.54	J/mol×K	758.14	Joback Method
cpg	629.29	J/mol×K	796.88	Joback Method

dvisc	0.0479580	Pa×s	244.76	Joback Method
dvisc	0.0051275	Pa×s	298.04	Joback Method
dvisc	0.0010801	Pa×s	351.32	Joback Method
dvisc	0.0003429	Pa×s	404.59	Joback Method
dvisc	0.0001422	Pa×s	457.87	Joback Method
dvisc	0.0000708	Pa×s	511.15	Joback Method
dvisc	0.0000402	Pa×s	564.43	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.20	K	0.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2986541&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

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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

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