2-Methoxyethoxycyclododecane (Ambrolignan)

Inchi: InChI=1S/C15H30O2/c1-3-17-15-13-11-9-7-5-4-6-8-10-12-14(15)16-2/h14-15H,3-13H2,1

InchiKey: QEESDNRMTAWNFQ-UHFFFAOYSA-N

Formula: C15H30O2

SMILES: CCOC1CCCCCCCCCCC1OC

Mol. weight [g/mol]: 242.40

Physical Properties

Property code	Value	Unit	Source
gf	-190.44	kJ/mol	Joback Method
hf	-620.35	kJ/mol	Joback Method
hfus	17.29	kJ/mol	Joback Method
hvap	54.96	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.321		Crippen Method
mcvol	223.090	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1750.20		NIST Webbook
rinpol	1762.80		NIST Webbook
rinpol	1779.20		NIST Webbook
rinpol	1750.20		NIST Webbook
rinpol	1762.80		NIST Webbook
rinpol	1779.20		NIST Webbook
ripol	2156.80		NIST Webbook
ripol	2156.80		NIST Webbook
ripol	2102.70		NIST Webbook
ripol	2127.80		NIST Webbook
ripol	2102.70		NIST Webbook
ripol	2127.80		NIST Webbook
tb	627.94	K	Joback Method
tc	848.73	K	Joback Method
tf	285.29	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.68	J/mol×K	627.94	Joback Method
cpg	753.87	J/mol×K	811.93	Joback Method
cpg	732.84	J/mol×K	775.14	Joback Method
cpg	710.06	J/mol×K	738.34	Joback Method
cpg	685.58	J/mol×K	701.54	Joback Method
cpg	659.44	J/mol×K	664.74	Joback Method
cpg	773.12	J/mol×K	848.73	Joback Method
dvisc	0.0000243	Pa×s	627.94	Joback Method
dvisc	0.0000400	Pa×s	570.83	Joback Method
dvisc	0.0000735	Pa×s	513.72	Joback Method
dvisc	0.0001573	Pa×s	456.62	Joback Method
dvisc	0.0004183	Pa×s	399.51	Joback Method
dvisc	0.0015414	Pa×s	342.40	Joback Method
dvisc	0.0095734	Pa×s	285.29	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R235722&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
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