Ethoxymethoxycyclododecane (Boisambrene)

Inchi: InChI=1S/C15H30O/c1-2-16-14-15-12-10-8-6-4-3-5-7-9-11-13-15/h15H,2-14H2,1H3
InchiKey: OGYDYKGQVKCZED-UHFFFAOYSA-N
Formula: C15H30O
SMILES: CCOCC1CCCCCCCCCCC1
Mol. weight [g/mol]: 226.40

Physical Properties

Property code	Value	Unit	Source
gf	-77.73	kJ/mol	Joback Method
hf	-467.79	kJ/mol	Joback Method
hfus	15.03	kJ/mol	Joback Method
hvap	52.86	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.944		Crippen Method
mcvol	217.220	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1735.90		NIST Webbook
rinpol	1718.30		NIST Webbook
rinpol	1704.20		NIST Webbook
ripol	2061.10		NIST Webbook
ripol	2001.50		NIST Webbook
ripol	2022.10		NIST Webbook
tb	610.19	K	Joback Method
tc	833.85	K	Joback Method
tf	267.30	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.91	J/mol×K	610.19	Joback Method
cpg	626.01	J/mol×K	647.47	Joback Method
cpg	652.45	J/mol×K	684.74	Joback Method
cpg	677.22	J/mol×K	722.02	Joback Method

cpg	700.30	J/mol×K	759.30	Joback Method
cpg	721.67	J/mol×K	796.57	Joback Method
cpg	741.32	J/mol×K	833.85	Joback Method
dvisc	0.0259074	Pa×s	267.30	Joback Method
dvisc	0.0030444	Pa×s	324.45	Joback Method
dvisc	0.0006794	Pa×s	381.60	Joback Method
dvisc	0.0002241	Pa×s	438.75	Joback Method
dvisc	0.0000954	Pa×s	495.89	Joback Method
dvisc	0.0000485	Pa×s	553.04	Joback Method
dvisc	0.0000280	Pa×s	610.19	Joback Method

Sources

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=R235757&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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