Ethoxymethoxycyclododecane (Buazambren)

Other names: (ethoxymethoxy)cyclododecane
Inchi: InChI=1S/C15H30O2/c1-2-16-14-17-15-12-10-8-6-4-3-5-7-9-11-13-15/h15H,2-14H2,1H3
InchiKey: VQNUNMBDOKEZHS-UHFFFAOYSA-N
Formula: C15H30O2
SMILES: CCOCOC1CCCCCCCCCCC1
Mol. weight [g/mol]: 242.40
CAS: 58567-11-6

Physical Properties

Property code	Value	Unit	Source
gf	-182.73	kJ/mol	Joback Method
hf	-600.01	kJ/mol	Joback Method
hfus	16.22	kJ/mol	Joback Method
hvap	55.27	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.670		Crippen Method
mcvol	223.090	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	1735.30		NIST Webbook
rinpol	1704.20		NIST Webbook
rinpol	1718.30		NIST Webbook
rinpol	1704.20		NIST Webbook
ripol	2061.10		NIST Webbook
ripol	2022.10		NIST Webbook
ripol	2001.50		NIST Webbook
tb	632.61	K	Joback Method
tc	853.39	K	Joback Method
tf	289.53	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	631.08	J/mol×K	632.61	Joback Method

cpg	750.51	J/mol×K	816.59	Joback Method
cpg	729.99	J/mol×K	779.80	Joback Method
cpg	707.76	J/mol×K	743.00	Joback Method
cpg	683.84	J/mol×K	706.20	Joback Method
cpg	658.27	J/mol×K	669.41	Joback Method
cpg	769.27	J/mol×K	853.39	Joback Method
dvisc	0.0000204	Pa×s	632.61	Joback Method
dvisc	0.0000347	Pa×s	575.43	Joback Method
dvisc	0.0000663	Pa×s	518.25	Joback Method
dvisc	0.0001485	Pa×s	461.07	Joback Method
dvisc	0.0004181	Pa×s	403.89	Joback Method
dvisc	0.0016564	Pa×s	346.71	Joback Method
dvisc	0.0113037	Pa×s	289.53	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58567116&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