2-(2-(2-Isopentoxy-ethoxy)-ethoxy)-ethanc

Inchi: InChI=1S/C13H28O5/c1-13(2)3-5-15-7-9-17-11-12-18-10-8-16-6-4-14/h13-14H,3-12H2,1
InchiKey: NNLUQPJLMQSXDD-UHFFFAOYSA-N
Formula: C13H28O5
SMILES: CC(C)CCOCCOCCOCCOCCO
Mol. weight [g/mol]: 264.36

Physical Properties

Property code	Value	Unit	Source
gf	-500.68	kJ/mol	Joback Method
hf	-998.04	kJ/mol	Joback Method
hfus	34.74	kJ/mol	Joback Method
hvap	70.46	kJ/mol	Joback Method
log10ws	-0.64		Crippen Method
logp	1.091		Crippen Method
mcvol	223.380	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	1896.70		NIST Webbook
rinpol	1896.70		NIST Webbook
tb	678.26	K	Joback Method
tc	842.32	K	Joback Method
tf	371.01	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.23	J/mol×K	678.26	Joback Method
cpg	661.34	J/mol×K	705.60	Joback Method
cpg	675.84	J/mol×K	732.95	Joback Method
cpg	689.71	J/mol×K	760.29	Joback Method
cpg	702.94	J/mol×K	787.63	Joback Method
cpg	715.53	J/mol×K	814.98	Joback Method
cpg	727.47	J/mol×K	842.32	Joback Method
dvisc	0.0018781	Pa×s	371.01	Joback Method

dvisc	0.0005458	Pa×s	422.22	Joback Method
dvisc	0.0002072	Pa×s	473.43	Joback Method
dvisc	0.0000950	Pa×s	524.63	Joback Method
dvisc	0.0000501	Pa×s	575.84	Joback Method
dvisc	0.0000293	Pa×s	627.05	Joback Method
dvisc	0.0000186	Pa×s	678.26	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R188537&Units=SI

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

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