2-[2-(2-Pentoxyethoxy)ethoxy]ethyl acetate

Other names: Triethylene glycol, pentyl ether, acetate
Inchi: InChI=1S/C13H26O5/c1-3-4-5-6-15-7-8-16-9-10-17-11-12-18-13(2)14/h3-12H2,1-2H3
InchiKey: LDNGEAUZTGLFNU-UHFFFAOYSA-N
Formula: C13H26O5
SMILES: CCCCCOCCOCCOCCOC(C)=O
Mol. weight [g/mol]: 262.34

Physical Properties

Property code	Value	Unit	Source
gf	-490.34	kJ/mol	Joback Method
hf	-953.11	kJ/mol	Joback Method
hfus	35.78	kJ/mol	Joback Method
hvap	60.92	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	1.789		Crippen Method
mcvol	219.080	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	1787.20		NIST Webbook
rinpol	1787.20		NIST Webbook
tb	640.39	K	Joback Method
tc	809.42	K	Joback Method
tf	375.12	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.19	J/mol×K	640.39	Joback Method
cpg	616.97	J/mol×K	668.56	Joback Method
cpg	632.13	J/mol×K	696.73	Joback Method
cpg	646.66	J/mol×K	724.90	Joback Method
cpg	660.55	J/mol×K	753.07	Joback Method
cpg	673.79	J/mol×K	781.25	Joback Method
cpg	686.35	J/mol×K	809.42	Joback Method

dvisc	0.0010023	Pa×s	375.12	Joback Method
dvisc	0.0005297	Pa×s	419.33	Joback Method
dvisc	0.0003162	Pa×s	463.54	Joback Method
dvisc	0.0002064	Pa×s	507.75	Joback Method
dvisc	0.0001443	Pa×s	551.97	Joback Method
dvisc	0.0001064	Pa×s	596.18	Joback Method
dvisc	0.0000818	Pa×s	640.39	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=R188651&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume