Triethylene glycol, nonyl ether, acetate

Other names: 2-(2-(2-nonyloxy-ethoxy)-ethoxy)-ethanol, acetate
Inchi: InChI=1S/C17H34O5/c1-3-4-5-6-7-8-9-10-19-11-12-20-13-14-21-15-16-22-17(2)18/h3-16
InchiKey: VKATUMXZADHLQW-UHFFFAOYSA-N
Formula: C17H34O5
SMILES: CCCCCCCCCOCCOCCOCCOC(C)=O
Mol. weight [g/mol]: 318.45

Physical Properties

Property code	Value	Unit	Source
gf	-456.66	kJ/mol	Joback Method
hf	-1035.67	kJ/mol	Joback Method
hfus	46.14	kJ/mol	Joback Method
hvap	69.82	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	3.350		Crippen Method
mcvol	275.440	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2187.50		NIST Webbook
rinpol	2187.50		NIST Webbook
tb	731.91	K	Joback Method
tc	903.97	K	Joback Method
tf	420.20	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.76	J/mol×K	731.91	Joback Method
cpg	844.59	J/mol×K	760.59	Joback Method
cpg	861.57	J/mol×K	789.26	Joback Method
cpg	877.67	J/mol×K	817.94	Joback Method
cpg	892.91	J/mol×K	846.61	Joback Method
cpg	907.27	J/mol×K	875.29	Joback Method
cpg	920.74	J/mol×K	903.97	Joback Method

dvisc	0.0007030	Pa×s	420.20	Joback Method
dvisc	0.0003516	Pa×s	472.15	Joback Method
dvisc	0.0002018	Pa×s	524.10	Joback Method
dvisc	0.0001280	Pa×s	576.05	Joback Method
dvisc	0.0000875	Pa×s	628.01	Joback Method
dvisc	0.0000634	Pa×s	679.96	Joback Method
dvisc	0.0000481	Pa×s	731.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R184337&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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