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

Other names: Triethylene glycol monobutyl ether, acetate
3,6,9-Trioxatridec-1-yl acetate
Inchi: InChI=1S/C12H24O5/c1-3-4-5-14-6-7-15-8-9-16-10-11-17-12(2)13/h3-11H2,1-2H3
InchiKey: SGQLKNKVOZVAAY-UHFFFAOYSA-N
Formula: C12H24O5
SMILES: CCCCOCCOCCOCCOC(C)=O
Mol. weight [g/mol]: 248.32

Physical Properties

Property code	Value	Unit	Source
gf	-498.76	kJ/mol	Joback Method
hf	-932.47	kJ/mol	Joback Method
hfus	33.19	kJ/mol	Joback Method
hvap	58.69	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	1.399		Crippen Method
mcvol	204.990	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	1627.30		NIST Webbook
rinpol	1627.30		NIST Webbook
rinpol	1690.00		NIST Webbook
tb	617.51	K	Joback Method
tc	786.87	K	Joback Method
tf	363.85	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.11	J/mol×K	617.51	Joback Method
cpg	563.27	J/mol×K	645.74	Joback Method
cpg	577.87	J/mol×K	673.96	Joback Method
cpg	591.90	J/mol×K	702.19	Joback Method
cpg	605.34	J/mol×K	730.42	Joback Method

cpg	618.17	J/mol×K	758.65	Joback Method
cpg	630.39	J/mol×K	786.87	Joback Method
dvisc	0.0010778	Pa×s	363.85	Joback Method
dvisc	0.0005785	Pa×s	406.13	Joback Method
dvisc	0.0003492	Pa×s	448.40	Joback Method
dvisc	0.0002299	Pa×s	490.68	Joback Method
dvisc	0.0001618	Pa×s	532.96	Joback Method
dvisc	0.0001198	Pa×s	575.23	Joback Method
dvisc	0.0000925	Pa×s	617.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351941&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume