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

Other names: Pentaethylene glycol monobutyl ether, acetate
3,6,9,12,15-Pentaoxanonadec-1-yl acetate

Inchi: InChI=1S/C16H32O7/c1-3-4-5-18-6-7-19-8-9-20-10-11-21-12-13-22-14-15-23-16(2)17/h3

InchiKey: XNPWMTYMHWZZES-UHFFFAOYSA-N

Formula: C16H32O7

SMILES: CCCCOCCOCCOCCOCCOCCOC(C)=O

Mol. weight [g/mol]: 336.42

Physical Properties

Property code	Value	Unit	Source
gf	-675.08	kJ/mol	Joback Method
hf	-1279.47	kJ/mol	Joback Method
hfus	45.92	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-0.82		Crippen Method
logp	1.433		Crippen Method
mcvol	273.090	ml/mol	McGowan Method
pc	1281.91	kPa	Joback Method
rinpol	2171.90		NIST Webbook
rinpol	2259.80		NIST Webbook
rinpol	2259.80		NIST Webbook
rinpol	2171.90		NIST Webbook
tb	753.87	K	Joback Method
tc	928.49	K	Joback Method
tf	453.39	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.53	J/mol×K	753.87	Joback Method
cpg	906.62	J/mol×K	899.38	Joback Method
cpg	893.31	J/mol×K	870.28	Joback Method
cpg	879.02	J/mol×K	841.18	Joback Method

cpg	863.77	J/mol×K	812.08	Joback Method
cpg	847.60	J/mol×K	782.97	Joback Method
cpg	918.94	J/mol×K	928.49	Joback Method
dvisc	0.0000315	Pa×s	753.87	Joback Method
dvisc	0.0000410	Pa×s	703.79	Joback Method
dvisc	0.0000556	Pa×s	653.71	Joback Method
dvisc	0.0000792	Pa×s	603.63	Joback Method
dvisc	0.0001205	Pa×s	553.55	Joback Method
dvisc	0.0001991	Pa×s	503.47	Joback Method
dvisc	0.0003677	Pa×s	453.39	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=U351940&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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