

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

Other names:	Tetraethylene glycol monobutyl ether, acetate 3,6,9,12-Tetraoxahexadec-1-yl acetate
Inchi:	InChI=1S/C14H28O6/c1-3-4-5-16-6-7-17-8-9-18-10-11-19-12-13-20-14(2)15/h3-13H2,1-14H
InchiKey:	XGPAKKIIHOORKP-UHFFFAOYSA-N
Formula:	C14H28O6
SMILES:	CCCCOCCOCCOCCOCCOC(C)=O
Mol. weight [g/mol]:	292.37

Physical Properties

Property code	Value	Unit	Source
gf	-586.92	kJ/mol	Joback Method
hf	-1105.97	kJ/mol	Joback Method
hfus	39.55	kJ/mol	Joback Method
hvap	65.55	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	1.416		Crippen Method
mcvol	239.040	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	1975.60		NIST Webbook
rinpol	1904.30		NIST Webbook
rinpol	1975.60		NIST Webbook
rinpol	1904.30		NIST Webbook
tb	685.69	K	Joback Method
tc	855.69	K	Joback Method
tf	408.62	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.44	J/molxK	685.69	Joback Method
cpg	701.66	J/molxK	714.02	Joback Method
cpg	717.18	J/molxK	742.36	Joback Method
cpg	731.98	J/molxK	770.69	Joback Method

cpg	746.05	J/molxK	799.02	Joback Method
cpg	759.35	J/molxK	827.36	Joback Method
cpg	771.89	J/molxK	855.69	Joback Method
dvisc	0.0006434	Paxs	408.62	Joback Method
dvisc	0.0003470	Paxs	454.80	Joback Method
dvisc	0.0002097	Paxs	500.98	Joback Method
dvisc	0.0001379	Paxs	547.15	Joback Method
dvisc	0.0000969	Paxs	593.33	Joback Method
dvisc	0.0000716	Paxs	639.51	Joback Method
dvisc	0.0000551	Paxs	685.69	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U351939&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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