1-((1-Butoxypropan-2-yl)oxy)propan-2-yl isobutyl carbonate

Inchi: InChI=1S/C15H30O5/c1-6-7-8-17-10-13(4)18-11-14(5)20-15(16)19-9-12(2)3/h12-14H,6-1

InchiKey: UFRIHVVHBRIZHF-UHFFFAOYSA-N

Formula: C15H30O5

SMILES: CCCCOCC(C)OCC(C)OC(=O)OCC(C)C

Mol. weight [g/mol]: 290.40

Physical Properties

Property code	Value	Unit	Source
gf	-480.82	kJ/mol	Joback Method
hf	-1010.23	kJ/mol	Joback Method
hfus	30.39	kJ/mol	Joback Method
hvap	64.21	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.406		Crippen Method
mcvol	247.260	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	1696.00		NIST Webbook
tb	684.83	K	Joback Method
tc	860.33	K	Joback Method
tf	352.66	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	712.85	J/mol×K	684.83	Joback Method
cpg	730.39	J/mol×K	714.08	Joback Method
cpg	747.13	J/mol×K	743.33	Joback Method
cpg	763.04	J/mol×K	772.58	Joback Method
cpg	778.13	J/mol×K	801.83	Joback Method
cpg	792.38	J/mol×K	831.08	Joback Method
cpg	805.78	J/mol×K	860.33	Joback Method
dvisc	0.0017244	Pa×s	352.66	Joback Method
dvisc	0.0006413	Pa×s	408.02	Joback Method

dvisc	0.0003021	Pa×s	463.38	Joback Method
dvisc	0.0001671	Pa×s	518.75	Joback Method
dvisc	0.0001036	Pa×s	574.11	Joback Method
dvisc	0.0000699	Pa×s	629.47	Joback Method
dvisc	0.0000502	Pa×s	684.83	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=U378306&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