

Isobutyl (1-propoxypropan-2-yl) carbonate

Inchi:	InChI=1S/C11H22O4/c1-5-6-13-8-10(4)15-11(12)14-7-9(2)3/h9-10H,5-8H2,1-4H3
InchiKey:	HTQLYHVCGUCEJS-UHFFFAOYSA-N
Formula:	C11H22O4
SMILES:	CCCOCC(C)OC(=O)OCC(C)C
Mol. weight [g/mol]:	218.29

Physical Properties

Property code	Value	Unit	Source
gf	-407.06	kJ/mol	Joback Method
hf	-790.17	kJ/mol	Joback Method
hfus	22.36	kJ/mol	Joback Method
hvap	53.28	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.611		Crippen Method
mcvol	185.030	ml/mol	McGowan Method
pc	1982.35	kPa	Joback Method
rinsol	1324.00		NIST Webbook
tb	571.33	K	Joback Method
tc	747.59	K	Joback Method
tf	300.35	K	Joback Method
vc	0.700	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.00	J/molxK	571.33	Joback Method
cpg	485.22	J/molxK	600.71	Joback Method
cpg	499.87	J/molxK	630.08	Joback Method
cpg	513.94	J/molxK	659.46	Joback Method
cpg	527.44	J/molxK	688.84	Joback Method
cpg	540.34	J/molxK	718.21	Joback Method
cpg	552.64	J/molxK	747.59	Joback Method
dvisc	0.0028826	Paxs	300.35	Joback Method
dvisc	0.0011893	Paxs	345.51	Joback Method

dvisc	0.0006021	Paxs	390.68	Joback Method
dvisc	0.0003510	Paxs	435.84	Joback Method
dvisc	0.0002265	Paxs	481.00	Joback Method
dvisc	0.0001575	Paxs	526.17	Joback Method
dvisc	0.0001160	Paxs	571.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378274&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mvol:	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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