

Isobutyl methyl carbonate

Inchi:

InChI=1S/C6H12O3/c1-5(2)4-9-6(7)8-3/h5H,4H2,1-3H3

InchiKey:

PDOXCFPUGNQQSW-UHFFFAOYSA-N

Formula:

C6H12O3

SMILES:

COC(=O)OCC(C)C

Mol. weight [g/mol]:

132.16

Physical Properties

Property code	Value	Unit	Source
gf	-341.72	kJ/mol	Joback Method
hf	-549.47	kJ/mol	Joback Method
hfus	11.75	kJ/mol	Joback Method
hvap	40.13	kJ/mol	Joback Method
log10ws	-1.02		Crippen Method
logp	1.425		Crippen Method
mcvol	108.710	ml/mol	McGowan Method
pc	3239.34	kPa	Joback Method
rinpol	857.30		NIST Webbook
tb	434.95	K	Joback Method
tc	616.32	K	Joback Method
tf	236.77	K	Joback Method
vc	0.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.96	J/mol×K	434.95	Joback Method
cpg	269.18	J/mol×K	586.09	Joback Method
cpg	260.32	J/mol×K	555.87	Joback Method
cpg	251.15	J/mol×K	525.64	Joback Method
cpg	241.69	J/mol×K	495.41	Joback Method
cpg	231.96	J/mol×K	465.18	Joback Method
cpg	277.74	J/mol×K	616.32	Joback Method
dvisc	0.0002290	Pa×s	434.95	Joback Method
dvisc	0.0002985	Pa×s	401.92	Joback Method

dvisc	0.0004081	Pa×s	368.89	Joback Method
dvisc	0.0005932	Pa×s	335.86	Joback Method
dvisc	0.0009358	Pa×s	302.83	Joback Method
dvisc	0.0016505	Pa×s	269.80	Joback Method
dvisc	0.0034104	Pa×s	236.77	Joback Method

Sources

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=U333939&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.chemeo.com/cid/30-631-7/isobutyl-methyl-carbonate.pdf>

Generated by Cheméo on 2025-12-24 08:19:10.549532506 +0000 UTC m=+6312548.079573161.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.