

Isobutyl (2-methoxyethyl) carbonate

Inchi:	InChI=1S/C8H16O4/c1-7(2)6-12-8(9)11-5-4-10-3/h7H,4-6H2,1-3H3
InchiKey:	OWZMVPOOMCGUHH-UHFFFAOYSA-N
Formula:	C8H16O4
SMILES:	COCCOC(=O)OCC(C)C
Mol. weight [g/mol]:	176.21

Physical Properties

Property code	Value	Unit	Source
gf	-429.88	kJ/mol	Joback Method
hf	-722.97	kJ/mol	Joback Method
hfus	18.12	kJ/mol	Joback Method
hvap	46.99	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	1.442		Crippen Method
mcvol	142.760	ml/mol	McGowan Method
pc	2587.22	kPa	Joback Method
rinsol	1154.00		NIST Webbook
tb	503.13	K	Joback Method
tc	680.70	K	Joback Method
tf	281.54	K	Joback Method
vc	0.537	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.22	J/molxK	503.13	Joback Method
cpg	340.49	J/molxK	532.73	Joback Method
cpg	352.40	J/molxK	562.32	Joback Method
cpg	363.94	J/molxK	591.92	Joback Method
cpg	375.08	J/molxK	621.51	Joback Method
cpg	385.82	J/molxK	651.11	Joback Method
cpg	396.14	J/molxK	680.70	Joback Method
dvisc	0.0024361	Paxs	281.54	Joback Method
dvisc	0.0012025	Paxs	318.47	Joback Method

dvisc	0.0006874	Paxs	355.40	Joback Method
dvisc	0.0004366	Paxs	392.34	Joback Method
dvisc	0.0002998	Paxs	429.27	Joback Method
dvisc	0.0002185	Paxs	466.20	Joback Method
dvisc	0.0001668	Paxs	503.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378283&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
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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