

Isopropyl (1-chloro-1-methylethyl) ether

Inchi:	InChI=1S/C6H13ClO/c1-5(2)8-6(3,4)7/h5H,1-4H3
InchiKey:	YHFGZATYFSSASH-UHFFFAOYSA-N
Formula:	C6H13ClO
SMILES:	CC(C)OC(C)(C)Cl
Mol. weight [g/mol]:	136.62

Physical Properties

Property code	Value	Unit	Source
gf	-116.89	kJ/mol	Joback Method
hf	-329.16	kJ/mol	Joback Method
hfus	5.74	kJ/mol	Joback Method
hvap	34.06	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.386		Crippen Method
mvol	113.510	ml/mol	McGowan Method
pc	3015.64	kPa	Joback Method
rinpol	798.00		NIST Webbook
rinpol	798.00		NIST Webbook
tb	392.86	K	Joback Method
tc	581.45	K	Joback Method
tf	196.95	K	Joback Method
vc	0.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.18	J/molxK	392.86	Joback Method
cpg	222.00	J/molxK	424.29	Joback Method
cpg	233.26	J/molxK	455.72	Joback Method
cpg	244.00	J/molxK	487.15	Joback Method
cpg	254.22	J/molxK	518.59	Joback Method
cpg	263.93	J/molxK	550.02	Joback Method
cpg	273.16	J/molxK	581.45	Joback Method
dvisc	0.0109013	Paxs	196.95	Joback Method

dvisc	0.0038341	Paxs	229.60	Joback Method
dvisc	0.0017493	Paxs	262.25	Joback Method
dvisc	0.0009495	Paxs	294.90	Joback Method
dvisc	0.0005822	Paxs	327.56	Joback Method
dvisc	0.0003901	Paxs	360.21	Joback Method
dvisc	0.0002793	Paxs	392.86	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=R629246&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

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