

Propyl 2-chloropropyl ether

Inchi:	InChI=1S/C6H13ClO/c1-3-4-8-5-6(2)7/h6H,3-5H2,1-2H3
InchiKey:	IWSSPFLMFCMBRR-UHFFFAOYSA-N
Formula:	C6H13ClO
SMILES:	CCCOCC(C)Cl
Mol. weight [g/mol]:	136.62

Physical Properties

Property code	Value	Unit	Source
gf	-119.73	kJ/mol	Joback Method
hf	-320.41	kJ/mol	Joback Method
hfus	13.16	kJ/mol	Joback Method
hvap	35.36	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	2.040		Crippen Method
mcvol	113.510	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	851.00		NIST Webbook
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tb	396.09	K	Joback Method
tc	572.75	K	Joback Method
tf	194.53	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.53	J/mol×K	396.09	Joback Method
cpg	218.94	J/mol×K	425.53	Joback Method
cpg	229.01	J/mol×K	454.98	Joback Method
cpg	238.74	J/mol×K	484.42	Joback Method
cpg	248.13	J/mol×K	513.86	Joback Method
cpg	257.18	J/mol×K	543.30	Joback Method
cpg	265.90	J/mol×K	572.75	Joback Method
dvisc	0.0059166	Pa×s	194.53	Joback Method

dvisc	0.0023735	Pa×s	228.12	Joback Method
dvisc	0.0012037	Pa×s	261.72	Joback Method
dvisc	0.0007124	Pa×s	295.31	Joback Method
dvisc	0.0004694	Pa×s	328.90	Joback Method
dvisc	0.0003341	Pa×s	362.50	Joback Method
dvisc	0.0002519	Pa×s	396.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R629419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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