

Propyl 3-chloropropyl ether

Inchi:	InChI=1S/C6H13ClO/c1-2-5-8-6-3-4-7/h2-6H2,1H3
InchiKey:	QODHJTGZDDJFDK-UHFFFAOYSA-N
Formula:	C6H13ClO
SMILES:	CCCOCCCCI
Mol. weight [g/mol]:	136.62

Physical Properties

Property code	Value	Unit	Source
gf	-117.29	kJ/mol	Joback Method
hf	-315.13	kJ/mol	Joback Method
hfus	16.68	kJ/mol	Joback Method
hvap	35.75	kJ/mol	Joback Method
log10ws	-1.57		Crippen Method
logp	2.042		Crippen Method
mvol	113.510	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	903.00		NIST Webbook
rinpol	903.00		NIST Webbook
tb	396.53	K	Joback Method
tc	569.18	K	Joback Method
tf	209.53	K	Joback Method
vc	0.439	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.56	J/molxK	396.53	Joback Method
cpg	218.65	J/molxK	425.30	Joback Method
cpg	228.41	J/molxK	454.08	Joback Method
cpg	237.86	J/molxK	482.85	Joback Method
cpg	246.99	J/molxK	511.63	Joback Method
cpg	255.80	J/molxK	540.40	Joback Method
cpg	264.30	J/molxK	569.18	Joback Method
dvisc	0.0036227	Paxs	209.53	Joback Method

dvisc	0.0017593	Paxs	240.70	Joback Method
dvisc	0.0010083	Paxs	271.86	Joback Method
dvisc	0.0006479	Paxs	303.03	Joback Method
dvisc	0.0004522	Paxs	334.20	Joback Method
dvisc	0.0003355	Paxs	365.36	Joback Method
dvisc	0.0002609	Paxs	396.53	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R629424&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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