

Propane, 1-(2-chloroethyl)-3-(1-propenyl)

Inchi:	InChI=1S/C8H15ClO2/c1-2-5-10-6-3-7-11-8-4-9/h2,5H,3-4,6-8H2,1H3/b5-2+
InchiKey:	CVSJNSVXNIDUCY-GORDUTHDSA-N
Formula:	C8H15ClO2
SMILES:	CC=COCCCOCCCI
Mol. weight [g/mol]:	178.66

Physical Properties

Property code	Value	Unit	Source
gf	-125.23	kJ/mol	Joback Method
hf	-371.41	kJ/mol	Joback Method
hfus	23.25	kJ/mol	Joback Method
hvap	42.56	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	2.182		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
rinsol	1685.00		NIST Webbook
tb	468.87	K	Joback Method
tc	647.26	K	Joback Method
tf	249.22	K	Joback Method
vc	0.548	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.39	J/molxK	468.87	Joback Method
cpg	350.79	J/molxK	617.53	Joback Method
cpg	340.57	J/molxK	587.80	Joback Method
cpg	329.92	J/molxK	558.07	Joback Method
cpg	318.84	J/molxK	528.33	Joback Method
cpg	307.33	J/molxK	498.60	Joback Method
cpg	360.60	J/molxK	647.26	Joback Method
dvisc	0.0001672	Paxs	468.87	Joback Method
dvisc	0.0002175	Paxs	432.26	Joback Method

dvisc	0.0002970	Paxs	395.65	Joback Method
dvisc	0.0004321	Paxs	359.05	Joback Method
dvisc	0.0006847	Paxs	322.44	Joback Method
dvisc	0.0012206	Paxs	285.83	Joback Method
dvisc	0.0025787	Paxs	249.22	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=R502344&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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