

2,2-Dichloropropyl propyl ether

Inchi:	InChI=1S/C6H12Cl2O/c1-3-4-9-5-6(2,7)8/h3-5H2,1-2H3
InchiKey:	BXUMLQQVHWVSBX-UHFFFAOYSA-N
Formula:	C6H12Cl2O
SMILES:	CCCOCC(C)(Cl)Cl
Mol. weight [g/mol]:	171.06

Physical Properties

Property code	Value	Unit	Source
gf	-126.38	kJ/mol	Joback Method
hf	-339.62	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	38.83	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.607		Crippen Method
mcvol	125.750	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	991.00		NIST Webbook
tb	430.73	K	Joback Method
tc	622.33	K	Joback Method
tf	241.87	K	Joback Method
vc	0.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.86	J/mol×K	430.73	Joback Method
cpg	286.74	J/mol×K	590.40	Joback Method
cpg	277.80	J/mol×K	558.46	Joback Method
cpg	268.36	J/mol×K	526.53	Joback Method
cpg	258.40	J/mol×K	494.60	Joback Method
cpg	247.91	J/mol×K	462.66	Joback Method
cpg	295.21	J/mol×K	622.33	Joback Method
dvisc	0.0002939	Paxs	430.73	Joback Method
dvisc	0.0003925	Paxs	399.25	Joback Method

dvisc	0.0005509	Paxs	367.78	Joback Method
dvisc	0.0008236	Paxs	336.30	Joback Method
dvisc	0.0013382	Paxs	304.82	Joback Method
dvisc	0.0024314	Paxs	273.35	Joback Method
dvisc	0.0051604	Paxs	241.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R629093&Units=SI

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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