2-Propyl-1-ol, dichloroacetate

Inchi: InChI=1S/C5H4Cl2O2/c1-2-3-9-5(8)4(6)7/h1,4H,3H2
InchiKey: ULEHAVSVSRGUEN-UHFFFAOYSA-N
Formula: C5H4Cl2O2
SMILES: C#CCOC(=O)C(Cl)Cl
Mol. weight [g/mol]: 166.99

Physical Properties

Property code	Value	Unit	Source
gf	-45.93	kJ/mol	Joback Method
hf	-136.19	kJ/mol	Joback Method
hfus	19.34	kJ/mol	Joback Method
hvap	44.12	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	0.966		Crippen Method
mcvol	104.630	ml/mol	McGowan Method
pc	4056.96	kPa	Joback Method
rinpol	962.00		NIST Webbook
rinpol	962.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	1720.00		NIST Webbook
tb	454.63	K	Joback Method
tc	666.28	K	Joback Method
tf	310.08	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	180.64	J/mol×K	454.63	Joback Method
cpg	186.89	J/mol×K	489.91	Joback Method
cpg	192.82	J/mol×K	525.18	Joback Method
cpg	198.43	J/mol×K	560.46	Joback Method
cpg	203.74	J/mol×K	595.73	Joback Method
cpg	208.74	J/mol×K	631.01	Joback Method

cpg	213.45	J/mol×K	666.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R26368&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

Legend

cpg:	Ideal gas heat capacity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume