2-Propyl-1-ol, chloroacetate

Inchi: InChI=1S/C5H5ClO2/c1-2-3-8-5(7)4-6/h1H,3-4H2
InchiKey: YVAMVRSKOCSBPY-UHFFFAOYSA-N
Formula: C5H5ClO2
SMILES: C#CCOC(=O)CCl
Mol. weight [g/mol]: 132.54

Physical Properties

Property code	Value	Unit	Source
gf	-31.56	kJ/mol	Joback Method
hf	-115.17	kJ/mol	Joback Method
hfus	18.66	kJ/mol	Joback Method
hvap	40.12	kJ/mol	Joback Method
log10ws	-0.73		Crippen Method
logp	0.402		Crippen Method
mcvol	92.390	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
rinpol	885.00		NIST Webbook
rinpol	885.00		NIST Webbook
ripol	1642.00		NIST Webbook
ripol	1642.00		NIST Webbook
tb	417.64	K	Joback Method
tc	617.44	K	Joback Method
tf	295.16	K	Joback Method
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	160.72	J/mol×K	417.64	Joback Method
cpg	167.05	J/mol×K	450.94	Joback Method
cpg	173.12	J/mol×K	484.24	Joback Method
cpg	178.92	J/mol×K	517.54	Joback Method
cpg	184.47	J/mol×K	550.84	Joback Method
cpg	189.76	J/mol×K	584.14	Joback Method

cpg	194.80	J/mol×K	617.44	Joback Method

Sources

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=R26354&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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