

1-Propen-2-ol, formate

Other names:	Isopropenyl formate
Inchi:	InChI=1S/C4H6O2/c1-4(2)6-3-5/h3H,1H2,2H3
InchiKey:	CAVPDPHVQVHXCQ-UHFFFAOYSA-N
Formula:	C4H6O2
SMILES:	C=C(C)OC=O
Mol. weight [g/mol]:	86.09
CAS:	32978-00-0

Physical Properties

Property code	Value	Unit	Source
gf	-142.43	kJ/mol	Joback Method
hf	-228.05	kJ/mol	Joback Method
hfus	7.00	kJ/mol	Joback Method
hvap	33.04	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.693		Crippen Method
mcvol	70.360	ml/mol	McGowan Method
pc	4456.32	kPa	Joback Method
ripol	905.00		NIST Webbook
tb	358.56	K	Joback Method
tc	539.87	K	Joback Method
tf	183.35	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	119.04	J/molxK	358.56	Joback Method
cpg	125.05	J/molxK	388.78	Joback Method
cpg	130.88	J/molxK	419.00	Joback Method
cpg	136.51	J/molxK	449.22	Joback Method
cpg	141.97	J/molxK	479.43	Joback Method
cpg	147.23	J/molxK	509.65	Joback Method
cpg	152.30	J/molxK	539.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32978000&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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