

Formic-d acid,ethylester

Inchi:	InChI=1S/C3H6O2/c1-2-5-3-4/h3H,2H2,1H3/i3D
InchiKey:	WBJINCZRORDGAQ-WFVSFCRTSA-N
Formula:	C3H5DO2
SMILES:	CCOC=O
Mol. weight [g/mol]:	75.08
CAS:	35976-76-2

Physical Properties

Property code	Value	Unit	Source
gf	-230.14	kJ/mol	Joback Method
hf	-323.05	kJ/mol	Joback Method
hfus	7.00	kJ/mol	Joback Method
hvap	31.40	kJ/mol	Joback Method
log10ws	0.06		Crippen Method
logp	0.179		Crippen Method
mcvol	60.570	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
tb	339.12	K	Joback Method
tc	513.09	K	Joback Method
tf	187.80	K	Joback Method
vc	0.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	101.20	J/molxK	339.12	Joback Method
cpg	125.25	J/molxK	484.09	Joback Method
cpg	120.65	J/molxK	455.10	Joback Method
cpg	115.94	J/molxK	426.10	Joback Method
cpg	111.13	J/molxK	397.11	Joback Method
cpg	106.21	J/molxK	368.11	Joback Method
cpg	129.73	J/molxK	513.09	Joback Method
dvisc	0.0002646	Paxs	339.12	Joback Method
dvisc	0.0003280	Paxs	313.90	Joback Method

dvisc	0.0004223	Paxs	288.68	Joback Method
dvisc	0.0005706	Paxs	263.46	Joback Method
dvisc	0.0008217	Paxs	238.24	Joback Method
dvisc	0.0012901	Paxs	213.02	Joback Method
dvisc	0.0022862	Paxs	187.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35976762&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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