

Formic acid, 2-propenyl ester

Other names:	2-Propenyl ester of formic acid Allyl formate Allylester kyseliny mravenci Formic acid, allyl ester UN 2336
Inchi:	InChI=1S/C4H6O2/c1-2-3-6-4-5/h2,4H,1,3H2
InchiKey:	ZHHZHHSFKCANOC-UHFFFAOYSA-N
Formula:	C4H6O2
SMILES:	C=CCOC=O
Mol. weight [g/mol]:	86.09
CAS:	1838-59-1

Physical Properties

Property code	Value	Unit	Source
gf	-133.88	kJ/mol	Joback Method
hf	-218.26	kJ/mol	Joback Method
hfus	8.31	kJ/mol	Joback Method
hvap	32.96	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	0.345		Crippen Method
mcvol	70.360	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
rinpol	571.00		NIST Webbook
rinpol	558.00		NIST Webbook
rinpol	550.00		NIST Webbook
rinpol	586.00		NIST Webbook
ripol	957.00		NIST Webbook
ripol	957.00		NIST Webbook
tb	358.68	K	Joback Method
tc	536.29	K	Joback Method
tf	197.31	K	Joback Method
vc	0.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.99	J/mol×K	358.68	Joback Method
cpg	146.81	J/mol×K	506.69	Joback Method
cpg	141.61	J/mol×K	477.09	Joback Method
cpg	136.22	J/mol×K	447.49	Joback Method
cpg	130.66	J/mol×K	417.88	Joback Method
cpg	124.92	J/mol×K	388.28	Joback Method
cpg	151.83	J/mol×K	536.29	Joback Method
dvisc	0.0002708	Pa×s	358.68	Joback Method
dvisc	0.0003346	Pa×s	331.78	Joback Method
dvisc	0.0004292	Pa×s	304.89	Joback Method
dvisc	0.0005778	Pa×s	278.00	Joback Method
dvisc	0.0008289	Pa×s	251.10	Joback Method
dvisc	0.0012966	Pa×s	224.20	Joback Method
dvisc	0.0022915	Pa×s	197.31	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.75191e+01
Coeff. B	-3.89041e+03
Coeff. C	-4.03260e+01
Temperature range (K), min.	266.10
Temperature range (K), max.	378.48

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=C1838591&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
pvap:	Vapor 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

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