

Formic acid, undecyl ester

Inchi:	InChI=1S/C12H24O2/c1-2-3-4-5-6-7-8-9-10-11-14-12-13/h12H,2-11H2,1H3
InchiKey:	OASFNORBKVGDRW-UHFFFAOYSA-N
Formula:	C12H24O2
SMILES:	CCCCCCCCCCCCOC=O
Mol. weight [g/mol]:	200.32

Physical Properties

Property code	Value	Unit	Source
gf	-154.36	kJ/mol	Joback Method
hf	-508.81	kJ/mol	Joback Method
hfus	30.31	kJ/mol	Joback Method
hvap	51.44	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.690		Crippen Method
mcvol	187.380	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinsol	1441.00		NIST Webbook
tb	545.04	K	Joback Method
tc	711.25	K	Joback Method
tf	289.23	K	Joback Method
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.26	J/molxK	545.04	Joback Method
cpg	535.20	J/molxK	683.55	Joback Method
cpg	522.15	J/molxK	655.84	Joback Method
cpg	508.54	J/molxK	628.14	Joback Method
cpg	494.36	J/molxK	600.44	Joback Method
cpg	479.60	J/molxK	572.74	Joback Method
cpg	547.71	J/molxK	711.25	Joback Method
dvisc	0.0002055	Paxs	545.04	Joback Method
dvisc	0.0002701	Paxs	502.40	Joback Method

dvisc	0.0003734	Paxs	459.77	Joback Method
dvisc	0.0005516	Paxs	417.13	Joback Method
dvisc	0.0008906	Paxs	374.50	Joback Method
dvisc	0.0016262	Paxs	331.87	Joback Method
dvisc	0.0035459	Paxs	289.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368250&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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